Revised phase transfer data in CAPRAM 3.0 rev

Species	$K_{H\,298}$, M atm^{-1}	-ΔH / R, K	reference	α	reference	D_g 10^5 m^2 s^{-1}	reference	Date
								08/2006
$CH_3CH_2CH(OH)$	135	7500	(Jayne, Duan et al. 1991)	0.011	(Jayne, Duan et al. 1991)	**0.97**	Fuller, 1986 [a)]	08/2006
$CH_3CH(OH)CH_3$	128	7400	(Jayne, Duan et al. 1991)	0.013	(Jayne, Duan et al. 1991)	**0.97**	Fuller, 1986 [a)]	08/2006
$CH_3CH_2CH_2CH(OH)$	130	7200	(Snider and Dawson 1985)	0.01		**0.85**	Fuller, 1986 [a)]	08/2006
$CH_3CH(OH)CH_2CH_3$	110	7300	(Snider and Dawson 1985)	0.01	Trend: smaller α with bigger compounds	**0.85**	Fuller, 1986 [a)]	08/2006
CH_3CH_2CHO	13	5700	(Zhou and Mopper 1990)	0.03	= α(CH_3CHO)	**1.00**	Fuller, 1986 [a)]	08/2006
$CH_3CH_2CH_2CHO$	9.6	6200	(Zhou and Mopper 1990)	0.03	= α(CH_3CH_2CHO)	**0.87**	Fuller, 1986 [a)]	08/2006
CH_3CH_2COOH	5710		(Khan, et al. 1995)	0.0322	= α(CH_3COOH)	**0.93**	Fuller, 1986 [a)]	08/2006
$CH_3CH_2CH_2COOH$	4700		(Khan et al., 1995)	0.0322	= α(CH_3COOH)	**0.82**	Fuller, 1986 [a)]	08/2006
$CH_3C(O)CHO$	1.4	**7541**	(Betterton and Hoffmann 1988)	0.03	= α(CH_3CHO)	**0.95**	Fuller, 1986 [a)]	08/2006
$CH_3C(O)CH_3$	32	5770	(Betterton 1991)	0.0054	(Schütze and Herrmann 2004)	**1.00**	Fuller, 1986 [a)]	08/2006
$CH_3C(O)CH_2CH_3$	19.8	2184	(Zhou and Mopper 1990)	0.0021	(Schütze and Herrmann 2004)	**0.87**	Fuller, 1986 [a)]	08/2006
HKET ⇌ $CH_3C(O)CH_2OH$	129		(Meylan and Howard, 1991)	0.008	= α(Aceton)	**0.96**	Fuller, 1986 [a)]	08/2006
DCB ⇌ OHCCH=CHCHO	$3\cdot10^5$		Estimated after the effective Henry constant of Glyoxal	0.023	= α(Glyoxal)	**0.86**	Fuller, 1986 [a)]	08/2006
$CH_3C(O)CH_2CH(CH_3)_2$	3.91		(Kim, Kalis et al. 2000)	0.01	estimated	**0.75**	Fuller, 1986 [a)]	08/2006
C_2H_5OCHO	2.59		(Bocek, 1976)	0.01	estimated	**0.93**	Fuller, 1986 [a)]	08/2006
$CH_2CH_2CH_2C(O)NCH_3$	$3.13\cdot10^5$		(Kim, Kalis et al. 2000)	0.01	estimated	**0.82**	Fuller, 1986 [a)]	08/2006
CH_2OHCHO	**4100**	**4630**	**(Betterton and Hoffmann, 1988)**	**0.04**	**= α(glycoldaldehyde)**	**1.10**	**Fuller, 1986 [a)]**	08/2006
CH_2OHCH_2OH	$4\cdot10^6$		(Bone, Cullis et al. 1983)	0.04	(Jayne, Duan et al. 1991)	**1.06**	Fuller, 1986 [a)]	08/2006

Remarks: revised and new values in bold; [a)] values calculated after the FSG method by Fuller, 1986

Revised reactions in CAPRAM 3.0 rev

Process in CAPRAM 3.0	Should be replaced by	Rate coefficients[(a)]	Reference	Comment	Date
	$HOOCC(O)COO^- \rightleftharpoons OOCC(O)COO^{2-} + H^+$	**$K = 1.64\cdot10^{-4}$; $k_{forw.} = 8.2\cdot10^6$ M^{-1} s^{-1}; $k_{back.} = 5\cdot10^{10}$ M^{-1} s^{-1}**	(Albalat, Claret et al. 1989)	Newly implemented	08/2006
	$OHCCH_2OH + H_2O \rightleftharpoons (OH)_2CHCH_2OH$	**$K = 1.64\cdot10^{-1}$; $k_{forw.} = 1.57\cdot10^{-3}$ M^{-1} s^{-1}; $k_{back.} = 9.60\cdot10^{-3}$ M^{-1} s^{-1}**	(Betterton and Hoffmann, 1988), k_{back} (Sorensen, 1972)	Newly implemented	08/2006

Remarks: [(a)] recommended values in bold

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