MPMC

Other names:	Xylylcarb
	Carbamic acid, methyl-, 3,4-xylyl ester
	Meobal
	MPMC
	V 17004
	3,4-Dimethylphenyl methylcarbamate
	3,4-Dimethylphenyl N-methylcarbamate
	3,4-Xylyl methylcarbamate
	3,4-Xylyl N-methylcarbamate
	Carbamic acid, N-methyl-, (3,4-dimethylphenyl) ester
	Methylcarbamic acid 3,4-xylyl ester
	S-1042
	Xylecarb
	3,4-Xylylester kyseliny methylkarbaminove
	Carbamic acid, 3,4-dimethylphenyl ester, N-methyl
	Phenol, 3,4-dimethyl-, 1-(N-methylcarbamate)
Inchi:	InChI=1S/C10H13NO2/c1-7-4-5-9(6-8(7)2)13-10(12)11-3/h4-6H,1-3H3,(H,11,12)
InchiKey:	WCJYTPVNMWIZCG-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CNC(=O)Oc1ccc(C)c(C)c1
Mol. weight [g/mol]:	179.22

Physical Properties

Property code	Value	Unit	Source
hfus	22.81	kJ/mol	Joback Method
log10ws	-2.78		Cheméo Relay (1.0)
logp	2.022		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
rinpol	1536.00		NIST Webbook
rinpol	1543.00		NIST Webbook
ripol	2132.00		NIST Webbook
ripol	2132.00		NIST Webbook
tb	536.35	K	Cheméo Relay (1.0)
tf	351.37 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.95	J/mol×K	591.30	Joback Method
cpg	360.01	J/mol×K	627.08	Joback Method
cpg	372.35	J/mol×K	662.86	Joback Method
cpg	383.98	J/mol×K	698.65	Joback Method
cpg	394.92	J/mol×K	734.43	Joback Method
cpg	405.16	J/mol×K	770.21	Joback Method
cpg	414.72	J/mol×K	805.99	Joback Method
hfust	24.97	kJ/mol	350.80	NIST Webbook
hfust	24.97	kJ/mol	350.80	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2425107&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point