2-Methylphenyl-n-methylcarbamate

Other names: Carbamic acid, N-methyl, 2-methylphenyl ester
Inchi: InChI=1S/C9H11NO2/c1-7-5-3-4-6-8(7)12-9(11)10-2/h3-6H,1-2H3,(H,10,11)
InchiKey: JDIMVGGWYBWUIS-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: CNC(=O)Oc1ccccc1C
Mol. weight [g/mol]: 165.19

Physical Properties

Property code	Value	Unit	Source
hfus	20.60	kJ/mol	Joback Method
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-1.81		Cheméo Relay (1.0)
logp	1.713		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
rinpol	1584.00		NIST Webbook
tb	516.46	K	Cheméo Relay (1.0)
tc	758.77	K	Cheméo Relay (1.0)
tf	320.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.19	J/mol×K	563.44	Joback Method
cpg	313.64	J/mol×K	599.68	Joback Method
cpg	325.37	J/mol×K	635.91	Joback Method
cpg	336.41	J/mol×K	672.15	Joback Method
cpg	346.75	J/mol×K	708.38	Joback Method
cpg	356.42	J/mol×K	744.62	Joback Method
cpg	365.43	J/mol×K	780.85	Joback Method

Sources

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=C1128785&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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