Carbamic acid, 4-methylphenyl, methyl ester

Inchi: InChI=1S/C9H11NO2/c1-7-3-5-8(6-4-7)10-9(11)12-2/h3-6H,1-2H3,(H,10,11)
InchiKey: OKBJVCWRESLMMD-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: COC(=O)Nc1ccc(C)cc1
Mol. weight [g/mol]: 165.19

Physical Properties

Property code	Value	Unit	Source
gf	-16.85	kJ/mol	Joback Method
hf	-195.36	kJ/mol	Joback Method
hfus	20.60	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.173		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1422.00		NIST Webbook
tb	563.44	K	Joback Method
tc	780.85	K	Joback Method
tf	354.95	K	Joback Method
vc	0.490	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R37884&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume