Carbamic acid, 3-chlorophenyl-, methyl ester

Inchi: InChI=1S/C8H8ClNO2/c1-12-8(11)10-7-4-2-3-6(9)5-7/h2-5H,1H3,(H,10,11)
InchiKey: SEPMCAVKHUPSMA-UHFFFAOYSA-N
Formula: C8H8ClNO2
SMILES: COC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 185.61

Physical Properties

Property code	Value	Unit	Source
gf	-37.20	kJ/mol	Joback Method
hf	-190.46	kJ/mol	Joback Method
hfus	22.21	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.518		Crippen Method
mcvol	129.480	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	1510.00		NIST Webbook
tb	577.99	K	Joback Method
tc	803.50	K	Joback Method
tf	373.60	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.88	J/mol×K	577.99	Joback Method
cpg	290.58	J/mol×K	615.58	Joback Method
cpg	300.59	J/mol×K	653.16	Joback Method
cpg	309.93	J/mol×K	690.75	Joback Method
cpg	318.62	J/mol×K	728.33	Joback Method
cpg	326.67	J/mol×K	765.92	Joback Method
cpg	334.09	J/mol×K	803.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U314750&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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