4-Chloro-m-cresol, isoBOC

Inchi: InChI=1S/C12H15ClO3/c1-8(2)7-15-12(14)16-10-4-5-11(13)9(3)6-10/h4-6,8H,7H2,1-3H3
InchiKey: AMVZTDGGEWZDNH-UHFFFAOYSA-N
Formula: C12H15ClO3
SMILES: Cc1cc(OC(=O)OCC(C)C)ccc1Cl
Mol. weight [g/mol]: 242.70

Physical Properties

Property code	Value	Unit	Source
gf	-209.98	kJ/mol	Joback Method
hf	-475.46	kJ/mol	Joback Method
hfus	24.75	kJ/mol	Joback Method
hvap	61.47	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.820		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
tb	646.30	K	Joback Method
tc	859.87	K	Joback Method
tf	385.77	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.19	J/mol×K	646.30	Joback Method
cpg	460.07	J/mol×K	681.89	Joback Method
cpg	473.16	J/mol×K	717.49	Joback Method
cpg	485.45	J/mol×K	753.08	Joback Method
cpg	496.94	J/mol×K	788.68	Joback Method
cpg	507.62	J/mol×K	824.27	Joback Method
cpg	517.51	J/mol×K	859.87	Joback Method
dvisc	0.0010947	Pa×s	385.77	Joback Method

dvisc	0.0006360	Pa×s	429.19	Joback Method
dvisc	0.0004082	Pa×s	472.61	Joback Method
dvisc	0.0002824	Pa×s	516.03	Joback Method
dvisc	0.0002068	Pa×s	559.46	Joback Method
dvisc	0.0001584	Pa×s	602.88	Joback Method
dvisc	0.0001258	Pa×s	646.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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