2,3-Dimethylphenol, isoBOC

Inchi: InChI=1S/C13H18O3/c1-9(2)8-15-13(14)16-12-7-5-6-10(3)11(12)4/h5-7,9H,8H2,1-4H3
InchiKey: HMJVGMQPGDOQSA-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: Cc1cccc(OC(=O)OCC(C)C)c1C
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	-189.63	kJ/mol	Joback Method
hf	-480.36	kJ/mol	Joback Method
hfus	23.14	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.475		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1584.00		NIST Webbook
tb	631.75	K	Joback Method
tc	838.47	K	Joback Method
tf	367.12	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.38	J/mol×K	631.75	Joback Method
cpg	484.79	J/mol×K	666.20	Joback Method
cpg	499.39	J/mol×K	700.66	Joback Method
cpg	513.17	J/mol×K	735.11	Joback Method
cpg	526.14	J/mol×K	769.57	Joback Method
cpg	538.30	J/mol×K	804.02	Joback Method
cpg	549.64	J/mol×K	838.47	Joback Method
dvisc	0.0011736	Pa×s	367.12	Joback Method
dvisc	0.0006555	Pa×s	411.23	Joback Method

dvisc	0.0004099	Pa×s	455.33	Joback Method
dvisc	0.0002784	Pa×s	499.44	Joback Method
dvisc	0.0002014	Pa×s	543.54	Joback Method
dvisc	0.0001529	Pa×s	587.64	Joback Method
dvisc	0.0001207	Pa×s	631.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R234927&Units=SI

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

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