

2,6-Dimethylphenol, isoBOC

Inchi:	InChI=1S/C13H18O3/c1-9(2)8-15-13(14)16-12-10(3)6-5-7-11(12)4/h5-7,9H,8H2,1-4H3
InchiKey:	PMPOWSQDHXMWJU-UHFFFAOYSA-N
Formula:	C13H18O3
SMILES:	Cc1cccc(C)c1OC(=O)OCC(C)C
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
rinsol	1504.00		NIST Webbook
tb	631.75	K	Joback Method
tc	838.47	K	Joback Method
tf	367.12	K	Joback Method
vc	0.692	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004099	Paxs	455.33	Joback Method
dvisc	0.0002784	Paxs	499.44	Joback Method
dvisc	0.0002014	Paxs	543.54	Joback Method
dvisc	0.0001529	Paxs	587.64	Joback Method
dvisc	0.0001207	Paxs	631.75	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=R234992&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

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