

2,3,6-Trimethylphenol, isoBOC

Inchi:	InChI=1S/C14H20O3/c1-9(2)8-16-14(15)17-13-11(4)7-6-10(3)12(13)5/h6-7,9H,8H2,1-5H
InchiKey:	VLEVACKHXDCWBQ-UHFFFAOYSA-N
Formula:	C14H20O3
SMILES:	Cc1ccc(C)c(OC(=O)OCC(C)C)c1C
Mol. weight [g/mol]:	236.31

Physical Properties

Property code	Value	Unit	Source
gf	-190.84	kJ/mol	Joback Method
hf	-512.47	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.783		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	659.61	K	Joback Method
tc	864.25	K	Joback Method
tf	390.91	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.49	J/molxK	659.61	Joback Method
cpg	591.12	J/molxK	830.15	Joback Method
cpg	578.67	J/molxK	796.04	Joback Method
cpg	565.38	J/molxK	761.93	Joback Method
cpg	551.25	J/molxK	727.82	Joback Method
cpg	536.29	J/molxK	693.72	Joback Method
cpg	602.73	J/molxK	864.25	Joback Method
dvisc	0.0001079	Paxs	659.61	Joback Method

dvisc	0.0001351	Paxs	614.83	Joback Method
dvisc	0.0001752	Paxs	570.04	Joback Method
dvisc	0.0002377	Paxs	525.26	Joback Method
dvisc	0.0003411	Paxs	480.48	Joback Method
dvisc	0.0005273	Paxs	435.69	Joback Method
dvisc	0.0009008	Paxs	390.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R234907&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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