

Orcinol, isoBOC

Inchi:	InChI=1S/C17H24O6/c1-11(2)9-20-16(18)22-14-6-13(5)7-15(8-14)23-17(19)21-10-12(3)
InchiKey:	NWKYDAUHKFHWOK-UHFFFAOYSA-N
Formula:	C17H24O6
SMILES:	<chem>Cc1cc(OC(=O)OCC(C)C)cc(OC(=O)OCC(C)C)c1</chem>
Mol. weight [g/mol]:	324.37

Physical Properties

Property code	Value	Unit	Source
gf	-497.31	kJ/mol	Joback Method
hf	-945.22	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	79.39	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.338		Crippen Method
mvol	253.250	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2166.00		NIST Webbook
tb	821.54	K	Joback Method
tc	1027.28	K	Joback Method
tf	491.59	K	Joback Method
vc	0.952	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.18	J/molxK	821.54	Joback Method
cpg	823.01	J/molxK	992.99	Joback Method
cpg	813.09	J/molxK	958.70	Joback Method
cpg	801.94	J/molxK	924.41	Joback Method
cpg	789.55	J/molxK	890.12	Joback Method
cpg	775.96	J/molxK	855.83	Joback Method
cpg	831.66	J/molxK	1027.28	Joback Method
dvisc	0.0000401	Paxs	821.54	Joback Method
dvisc	0.0000516	Paxs	766.55	Joback Method

dvisc	0.0000691	Paxs	711.56	Joback Method
dvisc	0.0000972	Paxs	656.57	Joback Method
dvisc	0.0001455	Paxs	601.57	Joback Method
dvisc	0.0002363	Paxs	546.58	Joback Method
dvisc	0.0004277	Paxs	491.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235311&Units=SI
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

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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