

1,2,4,5,7,8-hexaoxacyclononane, 3,3-dimethyl, 6,6,9,9-tetraethyl

Inchi:	InChI=1S/C13H26O6/c1-7-12(8-2)16-14-11(5,6)15-17-13(9-3,10-4)19-18-12/h7-10H2,1-6
InchiKey:	QSXXZBOBWQYNFW-UHFFFAOYSA-N
Formula:	C13H26O6
SMILES:	CCC1(CC)OOC(C)(C)OOC(CC)(CC)OO1
Mol. weight [g/mol]:	278.34

Physical Properties

Property code	Value	Unit	Source
gf	-501.88	kJ/mol	Joback Method
hf	-1062.77	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.613		Crippen Method
mcvol	218.390	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1418.40		NIST Webbook
rinpol	1413.90		NIST Webbook
rinpol	1404.80		NIST Webbook
rinpol	1420.90		NIST Webbook
rinpol	1418.40		NIST Webbook
rinpol	1421.70		NIST Webbook
rinpol	1404.80		NIST Webbook
rinpol	1410.30		NIST Webbook
rinpol	1418.00		NIST Webbook
tb	682.28	K	Joback Method
tc	905.05	K	Joback Method
tf	455.73	K	Joback Method
vc	0.790	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.08	J/mol×K	682.28	Joback Method

cpg	679.28	J/mol×K	719.41	Joback Method
cpg	698.95	J/mol×K	756.54	Joback Method
cpg	718.33	J/mol×K	793.67	Joback Method
cpg	737.69	J/mol×K	830.80	Joback Method
cpg	757.29	J/mol×K	867.93	Joback Method
cpg	777.38	J/mol×K	905.05	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=R419846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
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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