

1,2,4,5,7,8-hexaoxacyclononane, 3,6,9-trimethyl, 3,6,9-triethyl

Inchi:	InChI=1S/C12H24O6/c1-7-10(4)13-15-11(5,8-2)17-18-12(6,9-3)16-14-10/h7-9H2,1-6H3
InchiKey:	KVWLLOIEGKLBPA-UHFFFAOYSA-N
Formula:	C12H24O6
SMILES:	CCC1(C)OOC(C)(CC)OOC(C)(CC)OO1
Mol. weight [g/mol]:	264.32

Physical Properties

Property code	Value	Unit	Source
gf	-510.30	kJ/mol	Joback Method
hf	-1042.13	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.223		Crippen Method
mcvol	204.300	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1374.30		NIST Webbook
rinpol	1370.30		NIST Webbook
rinpol	1361.40		NIST Webbook
rinpol	1371.10		NIST Webbook
rinpol	1368.60		NIST Webbook
rinpol	1352.90		NIST Webbook
rinpol	1353.10		NIST Webbook
tb	659.40	K	Joback Method
tc	886.27	K	Joback Method
tf	444.46	K	Joback Method
vc	0.735	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.75	J/mol×K	659.40	Joback Method
cpg	624.37	J/mol×K	697.21	Joback Method
cpg	643.35	J/mol×K	735.02	Joback Method

cpg	661.96	J/mol×K	772.84	Joback Method
cpg	680.48	J/mol×K	810.65	Joback Method
cpg	699.16	J/mol×K	848.46	Joback Method
cpg	718.30	J/mol×K	886.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419851&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
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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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