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

Inchi: InChI=1S/C15H30O6/c1-7-13(8-2)16-18-14(9-3,10-4)20-21-15(11-5,12-6)19-17-13/h7-12

InchiKey: WYEDBMPUQDXWEF-UHFFFAOYSA-N

Formula: C15H30O6

SMILES: CCC1(CC)OOC(CC)(CC)OOC(CC)(CC)OO1

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-485.04	kJ/mol	Joback Method
hf	-1104.05	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	72.92	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.393		Crippen Method
mcvol	246.570	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	1569.20		NIST Webbook
rinpol	1569.70		NIST Webbook
rinpol	1572.60		NIST Webbook
rinpol	1569.50		NIST Webbook
rinpol	1568.90		NIST Webbook
rinpol	1569.50		NIST Webbook
rinpol	1568.90		NIST Webbook
rinpol	1544.20		NIST Webbook
rinpol	1564.60		NIST Webbook
tb	728.04	K	Joback Method
tc	943.80	K	Joback Method
tf	478.27	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.92	J/mol×K	728.04	Joback Method

cpg	793.30	J/mol×K	764.00	Joback Method
cpg	814.34	J/mol×K	799.96	Joback Method
cpg	835.25	J/mol×K	835.92	Joback Method
cpg	856.30	J/mol×K	871.88	Joback Method
cpg	877.73	J/mol×K	907.84	Joback Method
cpg	899.77	J/mol×K	943.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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