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

Inchi: InChI=1S/C11H22O6/c1-7-11(8-2)16-14-9(3,4)12-13-10(5,6)15-17-11/h7-8H2,1-6H3
InchiKey: DEAVANREEHNQGL-UHFFFAOYSA-N
Formula: C11H22O6
SMILES: CCC1(CC)OOC(C)(C)OOC(C)(C)OO1
Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	-518.72	kJ/mol	Joback Method
hf	-1021.49	kJ/mol	Joback Method
hfus	40.90	kJ/mol	Joback Method
hvap	64.01	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.833		Crippen Method
mcvol	190.210	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1269.50		NIST Webbook
rinpol	1270.90		NIST Webbook
rinpol	1275.70		NIST Webbook
rinpol	1270.40		NIST Webbook
rinpol	1268.80		NIST Webbook
rinpol	1273.10		NIST Webbook
rinpol	1257.10		NIST Webbook
tb	636.52	K	Joback Method
tc	867.83	K	Joback Method
tf	433.19	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.86	J/mol×K	636.52	Joback Method
cpg	570.88	J/mol×K	675.07	Joback Method
cpg	589.16	J/mol×K	713.62	Joback Method

cpg	606.99	J/mol×K	752.18	Joback Method
cpg	624.64	J/mol×K	790.73	Joback Method
cpg	642.40	J/mol×K	829.28	Joback Method
cpg	660.55	J/mol×K	867.83	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R419831&Units=SI

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