1,2,4,5-tetraoxacyclohexane, 3,6-dimethyl, 3,6-diethyl

Inchi: InChI=1S/C8H16O4/c1-5-7(3)9-11-8(4,6-2)12-10-7/h5-6H2,1-4H3
InchiKey: DYDYIBSLXXUTQU-UHFFFAOYSA-N
Formula: C8H16O4
SMILES: CCC1(C)OOC(C)(CC)OO1
Mol. weight [g/mol]: 176.21

Physical Properties

Property code	Value	Unit	Source
gf	-322.24	kJ/mol	Joback Method
hf	-671.99	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	49.26	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.149		Crippen Method
mcvol	136.200	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1059.40		NIST Webbook
rinpol	1046.90		NIST Webbook
rinpol	1080.80		NIST Webbook
rinpol	1085.60		NIST Webbook
rinpol	1072.80		NIST Webbook
rinpol	1063.30		NIST Webbook
rinpol	1057.80		NIST Webbook
tb	505.60	K	Joback Method
tc	721.53	K	Joback Method
tf	337.14	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.10	J/mol×K	505.60	Joback Method
cpg	355.64	J/mol×K	541.59	Joback Method
cpg	370.08	J/mol×K	577.58	Joback Method

cpg	383.58	J/mol×K	613.57	Joback Method
cpg	396.32	J/mol×K	649.56	Joback Method
cpg	408.48	J/mol×K	685.54	Joback Method
cpg	420.23	J/mol×K	721.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419891&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

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