1,2,4,5-tetraoxacyclohexane, 3,3,6,6-tetraethyl

Inchi: InChI=1S/C10H20O4/c1-5-9(6-2)11-13-10(7-3,8-4)14-12-9/h5-8H2,1-4H3
InchiKey: VGCWOVJYNWNYIM-UHFFFAOYSA-N
Formula: C10H20O4
SMILES: CCC1(CC)OOC(CC)(CC)OO1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	-305.40	kJ/mol	Joback Method
hf	-713.27	kJ/mol	Joback Method
hfus	33.88	kJ/mol	Joback Method
hvap	53.71	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.929		Crippen Method
mcvol	164.380	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1227.30		NIST Webbook
rinpol	1238.60		NIST Webbook
rinpol	1237.30		NIST Webbook
rinpol	1229.60		NIST Webbook
rinpol	1240.10		NIST Webbook
rinpol	1245.90		NIST Webbook
rinpol	1238.20		NIST Webbook
tb	551.36	K	Joback Method
tc	760.44	K	Joback Method
tf	359.68	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.52	J/mol×K	551.36	Joback Method
cpg	450.36	J/mol×K	586.21	Joback Method
cpg	466.21	J/mol×K	621.05	Joback Method

cpg	481.21	J/mol×K	655.90	Joback Method
cpg	495.55	J/mol×K	690.74	Joback Method
cpg	509.39	J/mol×K	725.59	Joback Method
cpg	522.89	J/mol×K	760.44	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=R419866&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