1,2,4,5-tetraoxacyclohexane, 3,6-dimethyl, 3,6-di-tertbutyl

Inchi: InChI=1S/C12H24O4/c1-9(2,3)11(7)13-15-12(8,16-14-11)10(4,5)6/h1-8H3
InchiKey: WKHNLQSJDUNPBS-UHFFFAOYSA-N
Formula: C12H24O4
SMILES: CC(C)(C)C1(C)OOC(C)(C(C)(C)C)OO1
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	-282.88	kJ/mol	Joback Method
hf	-772.05	kJ/mol	Joback Method
hfus	24.23	kJ/mol	Joback Method
hvap	55.57	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.421		Crippen Method
mcvol	192.560	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1347.20		NIST Webbook
rinpol	1355.40		NIST Webbook
rinpol	1340.40		NIST Webbook
rinpol	1342.80		NIST Webbook
rinpol	1335.10		NIST Webbook
rinpol	1331.20		NIST Webbook
rinpol	1333.50		NIST Webbook
tb	590.66	K	Joback Method
tc	818.64	K	Joback Method
tf	387.06	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.26	J/mol×K	590.66	Joback Method
cpg	559.30	J/mol×K	628.66	Joback Method
cpg	577.99	J/mol×K	666.65	Joback Method

cpg	595.60	J/mol×K	704.65	Joback Method
cpg	612.41	J/mol×K	742.65	Joback Method
cpg	628.69	J/mol×K	780.65	Joback Method
cpg	644.70	J/mol×K	818.64	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R419900&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