

Decalinhydroperoxide

Inchi: InChI=1S/C10H18O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h9,11H,1-8H2
InchiKey: HKLZOALUTLRUOI-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: OOC12CCCCC1CCCC2
Mol. weight [g/mol]: 170.25
CAS: 4181-83-3

Physical Properties

Property code	Value	Unit	Source
chs	-6158.40	kJ/mol	NIST Webbook
gf	-140.89	kJ/mol	Joback Method
hf	-397.98	kJ/mol	Joback Method
hfs	-348.00	kJ/mol	NIST Webbook
hfus	8.50	kJ/mol	Joback Method
hvap	56.31	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.979		Crippen Method
mcvol	141.780	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
tb	573.60	K	Joback Method
tc	786.12	K	Joback Method
tf	331.21	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.80	J/molxK	573.60	Joback Method
cpg	399.16	J/molxK	609.02	Joback Method
cpg	415.47	J/molxK	644.44	Joback Method
cpg	430.82	J/molxK	679.86	Joback Method
cpg	445.35	J/molxK	715.28	Joback Method
cpg	459.17	J/molxK	750.70	Joback Method
cpg	472.40	J/molxK	786.12	Joback Method

Sources

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=C4181833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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