2,5-Dimethyl-2-oxy-5-tert-butylperoxyhexane

Inchi: InChI=1S/C12H26O3/c1-10(2,3)14-15-12(6,7)9-8-11(4,5)13/h13H,8-9H2,1-7H3
InchiKey: WVYJQAHQPIRIIP-UHFFFAOYSA-N
Formula: C12H26O3
SMILES: CC(C)(O)CCC(C)(C)OOC(C)(C)C
Mol. weight [g/mol]: 218.33
CAS: 87047-20-9

Physical Properties

Property code	Value	Unit	Source
chl	-7741.00 ± 2.20	kJ/mol	NIST Webbook
gf	-288.14	kJ/mol	Joback Method
hf	-620.60 ± 2.20	kJ/mol	NIST Webbook
hfl	-695.90 ± 2.20	kJ/mol	NIST Webbook
hfus	11.06	kJ/mol	Joback Method
hvap	75.30 ± 0.10	kJ/mol	NIST Webbook
log10ws	-3.61		Crippen Method
logp	3.063		Crippen Method
mcvol	197.550	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
tb	601.29	K	Joback Method
tc	781.71	K	Joback Method
tf	337.54	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.38	J/mol×K	601.29	Joback Method
cpg	615.71	J/mol×K	751.64	Joback Method
cpg	602.83	J/mol×K	721.57	Joback Method
cpg	589.20	J/mol×K	691.50	Joback Method
cpg	574.77	J/mol×K	661.43	Joback Method
cpg	559.52	J/mol×K	631.36	Joback Method
cpg	627.87	J/mol×K	781.71	Joback Method

dvisc	0.0000339	Pa×s	601.29	Joback Method
dvisc	0.0000582	Pa×s	557.33	Joback Method
dvisc	0.0001096	Pa×s	513.37	Joback Method
dvisc	0.0002327	Pa×s	469.41	Joback Method
dvisc	0.0005770	Pa×s	425.46	Joback Method
dvisc	0.0017637	Pa×s	381.50	Joback Method
dvisc	0.0072123	Pa×s	337.54	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=C87047209&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid 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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