2,5-Dimethyl-2-hydroperoxide-5-tert-butylperoxyh

Inchi: InChI=1S/C12H26O4/c1-10(2,3)15-16-12(6,7)9-8-11(4,5)14-13/h13H,8-9H2,1-7H3
InchiKey: LMYXBQKXPSZHAH-UHFFFAOYSA-N
Formula: C12H26O4
SMILES: CC(C)(C)OOC(C)(C)CCC(C)(C)OO
Mol. weight [g/mol]: 234.33
CAS: 23661-84-9

Physical Properties

Property code	Value	Unit	Source
chl	-7801.90 ± 3.30	kJ/mol	NIST Webbook
gf	-393.14	kJ/mol	Joback Method
hf	-561.80 ± 3.30	kJ/mol	NIST Webbook
hfl	-636.00 ± 3.30	kJ/mol	NIST Webbook
hfus	12.25	kJ/mol	Joback Method
hvap	74.20 ± 0.20	kJ/mol	NIST Webbook
log10ws	-3.75		Crippen Method
logp	3.560		Crippen Method
mcvol	203.420	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
tb	623.71	K	Joback Method
tc	803.50	K	Joback Method
tf	359.77	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.46	J/mol×K	623.71	Joback Method
cpg	587.23	J/mol×K	653.67	Joback Method
cpg	602.17	J/mol×K	683.64	Joback Method
cpg	616.30	J/mol×K	713.60	Joback Method
cpg	629.67	J/mol×K	743.57	Joback Method
cpg	642.29	J/mol×K	773.53	Joback Method
cpg	654.21	J/mol×K	803.50	Joback Method

dvisc	0.0034716	Pa×s	359.77	Joback Method
dvisc	0.0009591	Pa×s	403.76	Joback Method
dvisc	0.0003412	Pa×s	447.75	Joback Method
dvisc	0.0001460	Pa×s	491.74	Joback Method
dvisc	0.0000718	Pa×s	535.73	Joback Method
dvisc	0.0000394	Pa×s	579.72	Joback Method
dvisc	0.0000235	Pa×s	623.71	Joback Method

Sources

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=C23661849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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