2,2-Bis(tert-butylperoxy) butane

Other names: 2,2-Bis(tert-butylperoxy) butane
Inchi: InChI=1S/C12H26O4/c1-9-12(8,15-13-10(2,3)4)16-14-11(5,6)7/h9H2,1-8H3
InchiKey: HQOVXPHOJANJBR-UHFFFAOYSA-N
Formula: C12H26O4
SMILES: CCC(C)(OOC(C)(C)C)OOC(C)(C)C
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
chl	-7821.20 ± 6.30	kJ/mol	NIST Webbook
hf	-571.01	kJ/mol	Cheméo Relay (1.0)
hfus	9.35	kJ/mol	Joback Method
ie	8.74	eV	Cheméo Relay (1.0)
logp	3.606		Crippen Method
mcvol	203.420	ml/mol	McGowan Method
tb	481.30	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.13	J/mol×K	553.95	Joback Method
cpg	628.19	J/mol×K	741.20	Joback Method
cpg	614.01	J/mol×K	709.99	Joback Method
cpg	598.99	J/mol×K	678.78	Joback Method
cpg	583.12	J/mol×K	647.57	Joback Method
cpg	566.37	J/mol×K	616.37	Joback Method
cpg	548.71	J/mol×K	585.16	Joback Method
dvisc	0.0002581	Pa×s	437.57	Joback Method
dvisc	0.0000723	Pa×s	553.95	Joback Method
dvisc	0.0001036	Pa×s	515.16	Joback Method
dvisc	0.0001576	Pa×s	476.36	Joback Method
dvisc	0.0023173	Pa×s	321.18	Joback Method
dvisc	0.0004652	Pa×s	398.77	Joback Method
dvisc	0.0009523	Pa×s	359.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2167239&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature