

Hexaneperoxoic acid, 2-ethyl-, 1,1-dimethylethyl ester

Other names:	tert-butyl 2-ethylperoxyhexanoate
Inchi:	InChI=1S/C12H24O3/c1-6-8-9-10(7-2)11(13)14-15-12(3,4)5/h10H,6-9H2,1-5H3
InchiKey:	WYKYCHHWIJXDAO-UHFFFAOYSA-N
Formula:	C12H24O3
SMILES:	CCCCC(CC)C(=O)OOC(C)(C)C
Mol. weight [g/mol]:	216.32
CAS:	3006-82-4

Physical Properties

Property code	Value	Unit	Source
gf	-288.36	kJ/mol	Joback Method
hf	-682.06	kJ/mol	Joback Method
hfus	19.87	kJ/mol	Joback Method
hvap	52.19	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.476		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
tb	569.00	K	Joback Method
tc	750.28	K	Joback Method
tf	306.81	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.31	J/molxK	569.00	Joback Method
cpg	570.95	J/molxK	720.06	Joback Method
cpg	557.27	J/molxK	689.85	Joback Method
cpg	542.88	J/molxK	659.64	Joback Method
cpg	527.77	J/molxK	629.43	Joback Method
cpg	511.92	J/molxK	599.21	Joback Method
cpg	583.93	J/molxK	750.28	Joback Method
dvisc	0.0001282	Paxs	569.00	Joback Method

dvisc	0.0001771	Paxs	525.30	Joback Method
dvisc	0.0002594	Paxs	481.60	Joback Method
dvisc	0.0004099	Paxs	437.90	Joback Method
dvisc	0.0007171	Paxs	394.21	Joback Method
dvisc	0.0014420	Paxs	350.51	Joback Method
dvisc	0.0035385	Paxs	306.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3006824&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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