2-Tert-pentylperoxyethanol

Inchi: InChI=1S/C7H16O3/c1-4-7(2,3)10-9-6-5-8/h8H,4-6H2,1-3H3
InchiKey: IMQAXPAGPCAQIU-UHFFFAOYSA-N
Formula: C7H16O3
SMILES: CCC(C)(C)OOCCO
Mol. weight [g/mol]: 148.20
CAS: 51452-08-5

Physical Properties

Property code	Value	Unit	Source
chl	-4507.00 ± 1.30	kJ/mol	NIST Webbook
gf	-436.29	kJ/mol	Joback Method
hf	-464.10 ± 3.00	kJ/mol	NIST Webbook
hfl	-534.20 ± 1.60	kJ/mol	NIST Webbook
hfus	14.93	kJ/mol	Joback Method
hvap	53.97	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.115		Crippen Method
mcvol	127.100	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	506.73	K	Joback Method
tc	682.92	K	Joback Method
tf	274.22	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.17	J/mol×K	506.73	Joback Method
cpg	298.99	J/mol×K	536.10	Joback Method
cpg	309.27	J/mol×K	565.46	Joback Method
cpg	319.03	J/mol×K	594.83	Joback Method
cpg	328.29	J/mol×K	624.19	Joback Method
cpg	337.06	J/mol×K	653.56	Joback Method
cpg	345.36	J/mol×K	682.92	Joback Method

dvisc	0.0344066	Pa×s	274.22	Joback Method
dvisc	0.0076863	Pa×s	312.97	Joback Method
dvisc	0.0023890	Pa×s	351.72	Joback Method
dvisc	0.0009364	Pa×s	390.48	Joback Method
dvisc	0.0004347	Pa×s	429.23	Joback Method
dvisc	0.0002291	Pa×s	467.98	Joback Method
dvisc	0.0001332	Pa×s	506.73	Joback Method
hvapt	70.10 ± 2.50	kJ/mol	290.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51452085&Units=SI
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

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
hvapt: Enthalpy of vaporization at a given temperature
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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