t-Butylperoxymethyloxirane

Inchi: InChI=1S/C7H14O3/c1-7(2,3)10-9-5-6-4-8-6/h6H,4-5H2,1-3H3
InchiKey: DFNGDRYVYUIBMK-UHFFFAOYSA-N
Formula: C7H14O3
SMILES: CC(C)(C)OOCC1CO1
Mol. weight [g/mol]: 146.18
CAS: 33415-52-0

Physical Properties

Property code	Value	Unit	Source
chl	-4436.00 ± 2.00	kJ/mol	NIST Webbook
chl	-4436.00 ± 2.00	kJ/mol	NIST Webbook
gf	-324.84	kJ/mol	Joback Method
hf	-265.20 ± 2.00	kJ/mol	NIST Webbook
hf	-265.20 ± 2.00	kJ/mol	NIST Webbook
hf	-267.50 ± 2.80	kJ/mol	NIST Webbook
hf	-272.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-319.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-319.00 ± 2.00	kJ/mol	NIST Webbook
hfus	16.95	kJ/mol	Joback Method
hvap	53.85 ± 0.39	kJ/mol	NIST Webbook
log10ws	-1.12		Crippen Method
logp	1.132		Crippen Method
mcvol	116.240	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
tb	448.24	K	Joback Method
tc	647.83	K	Joback Method
tf	257.91	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.77	J/mol×K	448.24	Joback Method
cpg	309.42	J/mol×K	614.56	Joback Method

cpg	299.03	J/mol×K	581.30	Joback Method
cpg	287.91	J/mol×K	548.03	Joback Method
cpg	276.02	J/mol×K	514.77	Joback Method
cpg	263.32	J/mol×K	481.50	Joback Method
cpg	319.11	J/mol×K	647.83	Joback Method
dvisc	0.0004961	Pa×s	448.24	Joback Method
dvisc	0.0006199	Pa×s	416.52	Joback Method
dvisc	0.0008035	Pa×s	384.80	Joback Method
dvisc	0.0010912	Pa×s	353.07	Joback Method
dvisc	0.0015743	Pa×s	321.35	Joback Method
dvisc	0.0024610	Pa×s	289.63	Joback Method
dvisc	0.0042940	Pa×s	257.91	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=C33415520&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