1,1,3-Trimethoxypropane

Inchi: InChI=1S/C6H14O3/c1-7-5-4-6(8-2)9-3/h6H,4-5H2,1-3H3
InchiKey: FKZYYYDRLJCHGL-UHFFFAOYSA-N
Formula: C6H14O3
SMILES: COCCC(OC)OC
Mol. weight [g/mol]: 134.17
CAS: 14315-97-0

Physical Properties

Property code	Value	Unit	Source
gf	-317.80	kJ/mol	Joback Method
hf	-569.11	kJ/mol	Joback Method
hfus	11.34	kJ/mol	Joback Method
hvap	35.79	kJ/mol	Joback Method
log10ws	-0.20		Crippen Method
logp	0.642		Crippen Method
mcvol	113.010	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
tb	403.50	K	Joback Method
tc	573.01	K	Joback Method
tf	209.07	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.23	J/mol×K	403.50	Joback Method
cpg	275.94	J/mol×K	544.76	Joback Method
cpg	266.60	J/mol×K	516.51	Joback Method
cpg	257.05	J/mol×K	488.25	Joback Method
cpg	247.29	J/mol×K	460.00	Joback Method
cpg	237.35	J/mol×K	431.75	Joback Method
cpg	285.05	J/mol×K	573.01	Joback Method
dvisc	0.0001738	Pa×s	403.50	Joback Method
dvisc	0.0002292	Pa×s	371.10	Joback Method

dvisc	0.0003188	Pa×s	338.69	Joback Method
dvisc	0.0004754	Pa×s	306.28	Joback Method
dvisc	0.0007793	Pa×s	273.88	Joback Method
dvisc	0.0014587	Pa×s	241.47	Joback Method
dvisc	0.0033162	Pa×s	209.07	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	326.50 ± 1.50	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14315970&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume