Alpha-monopropionin

Other names: 1-Mono propionin
(dl) glycerol 1-propionate
Inchi: InChI=1S/C6H12O4/c1-2-6(9)10-4-5(8)3-7/h5,7-8H,2-4H2,1H3
InchiKey: AALUCPRYHRPMAG-UHFFFAOYSA-N
Formula: C6H12O4
SMILES: CCC(=O)OCC(O)CO
Mol. weight [g/mol]: 148.16
CAS: 624-47-5

Physical Properties

Property code	Value	Unit	Source
gf	-510.36	kJ/mol	Joback Method
hf	-721.71	kJ/mol	Joback Method
hfus	18.74	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	0.16		Crippen Method
logp	-0.707		Crippen Method
mcvol	114.580	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
tb	596.89	K	Joback Method
tc	765.41	K	Joback Method
tf	336.18	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.26	J/mol×K	596.89	Joback Method
cpg	298.25	J/mol×K	624.98	Joback Method
cpg	305.91	J/mol×K	653.06	Joback Method
cpg	313.24	J/mol×K	681.15	Joback Method
cpg	320.25	J/mol×K	709.24	Joback Method
cpg	326.94	J/mol×K	737.33	Joback Method
cpg	333.30	J/mol×K	765.41	Joback Method

dvisc	0.0159133	Pa×s	336.18	Joback Method
dvisc	0.0031897	Pa×s	379.63	Joback Method
dvisc	0.0008894	Pa×s	423.08	Joback Method
dvisc	0.0003146	Pa×s	466.53	Joback Method
dvisc	0.0001329	Pa×s	509.99	Joback Method
dvisc	0.0000642	Pa×s	553.44	Joback Method
dvisc	0.0000345	Pa×s	596.89	Joback Method
hvapt	75.80	kJ/mol	422.00	NIST Webbook

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=C624475&Units=SI

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
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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