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	333.30	J/mol×K	765.41	Joback Method
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

dvisc	0.0000345	Pa×s	596.89	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
hvapt	75.80	kJ/mol	422.00	NIST Webbook

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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