2-propoxy-1-propanol

Inchi: InChI=1S/C6H14O2/c1-3-4-8-6(2)5-7/h6-7H,3-5H2,1-2H3
InchiKey: PSKIVCBTSGNKBB-UHFFFAOYSA-N
Formula: C6H14O2
SMILES: CCCOC(C)CO
Mol. weight [g/mol]: 118.17

Physical Properties

Property code	Value	Unit	Source
gf	-244.62	kJ/mol	Joback Method
hf	-456.90	kJ/mol	Joback Method
hfus	13.05	kJ/mol	Joback Method
hvap	47.65	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.794		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	855.60		NIST Webbook
rinpol	855.60		NIST Webbook
ripol	1323.20		NIST Webbook
ripol	1323.20		NIST Webbook
tb	450.84	K	Joback Method
tc	615.45	K	Joback Method
tf	225.43	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.32	J/mol×K	450.84	Joback Method
cpg	239.95	J/mol×K	478.28	Joback Method
cpg	249.26	J/mol×K	505.71	Joback Method
cpg	258.28	J/mol×K	533.15	Joback Method
cpg	266.99	J/mol×K	560.58	Joback Method
cpg	275.39	J/mol×K	588.02	Joback Method

cpg	283.50	J/mol×K	615.45	Joback Method
dvisc	0.0820702	Pa×s	225.43	Joback Method
dvisc	0.0143235	Pa×s	263.00	Joback Method
dvisc	0.0038675	Pa×s	300.57	Joback Method
dvisc	0.0013969	Pa×s	338.13	Joback Method
dvisc	0.0006185	Pa×s	375.70	Joback Method
dvisc	0.0003176	Pa×s	413.27	Joback Method
dvisc	0.0001822	Pa×s	450.84	Joback Method

Sources

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=R206358&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume