Glycidyl butyrate

Inchi: InChI=1S/C7H12O3/c1-2-3-7(8)10-5-6-4-9-6/h6H,2-5H2,1H3
InchiKey: YLNSNVGRSIOCEU-UHFFFAOYSA-N
Formula: C7H12O3
SMILES: CCCC(=O)OCC1CO1
Mol. weight [g/mol]: 144.17
CAS: 2461-40-7

Physical Properties

Property code	Value	Unit	Source
chl	-3909.20 ± 4.20	kJ/mol	NIST Webbook
gf	-251.23	kJ/mol	Joback Method
hf	-501.70 ± 2.80	kJ/mol	NIST Webbook
hfl	-560.40 ± 4.20	kJ/mol	NIST Webbook
hfus	22.79	kJ/mol	Joback Method
hvap	58.00 ± 0.40	kJ/mol	NIST Webbook
hvap	58.67 ± 0.35	kJ/mol	NIST Webbook
hvap	58.70 ± 0.40	kJ/mol	NIST Webbook
hvap	58.00 ± 0.42	kJ/mol	NIST Webbook
log10ws	-0.71		Crippen Method
logp	0.728		Crippen Method
mcvol	111.940	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	469.54	K	Joback Method
tc	660.17	K	Joback Method
tf	285.32	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.90	J/mol×K	660.17	Joback Method
cpg	251.76	J/mol×K	469.54	Joback Method
cpg	263.66	J/mol×K	501.31	Joback Method
cpg	274.98	J/mol×K	533.08	Joback Method

cpg	285.75	J/mol×K	564.85	Joback Method
cpg	295.98	J/mol×K	596.62	Joback Method
cpg	305.69	J/mol×K	628.39	Joback Method
dvisc	0.0005265	Pa×s	469.54	Joback Method
dvisc	0.0022275	Pa×s	285.32	Joback Method
dvisc	0.0015585	Pa×s	316.02	Joback Method
dvisc	0.0011616	Pa×s	346.73	Joback Method
dvisc	0.0009082	Pa×s	377.43	Joback Method
dvisc	0.0007369	Pa×s	408.13	Joback Method
dvisc	0.0006156	Pa×s	438.84	Joback Method
rfi	1.42900		298.15	Isobaric (vapour-liquid) equilibria data for the binary system of glycidyl butyrate (1) and epichlorohydrin (2) at 100 kPa,88.66 kPa,56 kPa

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isobaric (vapour-liquid) equilibria data for the binary system of glycidyl butyrate (1) and epichlorohydrin (2) at 100 kPa,88.66 kPa,56 kPa:	https://www.doi.org/10.1016/j.jct.2012.01.005
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=C2461407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rfi:	Refractive Index
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume