Glycerol monoacetate

Other names: glycerol acetate
Monoacetine
Inchi: InChI=1S/C5H10O4/c1-4(7)9-3-5(8)2-6/h5-6,8H,2-3H2,1H3
InchiKey: KMZHZAAOEWVPSE-UHFFFAOYSA-N
Formula: C5H10O4
SMILES: CC(=O)OCC(O)CO
Mol. weight [g/mol]: 134.13
CAS: 26446-35-5

Physical Properties

Property code	Value	Unit	Source
chl	-2487.50 ± 3.70	kJ/mol	NIST Webbook
gf	-518.78	kJ/mol	Joback Method
hf	-701.07	kJ/mol	Joback Method
hfl	-903.53	kJ/mol	NIST Webbook
hfus	16.15	kJ/mol	Joback Method
hvap	68.85	kJ/mol	Joback Method
log10ws	0.58		Crippen Method
logp	-1.097		Crippen Method
mcvol	100.490	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
tb	574.01	K	Joback Method
tc	743.34	K	Joback Method
tf	324.91	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.56	J/mol×K	574.01	Joback Method
cpg	278.12	J/mol×K	715.12	Joback Method
cpg	272.16	J/mol×K	686.90	Joback Method
cpg	265.93	J/mol×K	658.68	Joback Method
cpg	259.42	J/mol×K	630.45	Joback Method
cpg	252.63	J/mol×K	602.23	Joback Method
cpg	283.79	J/mol×K	743.34	Joback Method
dvisc	0.0000444	Pa×s	574.01	Joback Method
dvisc	0.0000832	Pa×s	532.49	Joback Method
dvisc	0.0001734	Pa×s	490.98	Joback Method
dvisc	0.0004140	Pa×s	449.46	Joback Method
dvisc	0.0011802	Pa×s	407.94	Joback Method
dvisc	0.0042658	Pa×s	366.43	Joback Method
dvisc	0.0214122	Pa×s	324.91	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26446355&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

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

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