Diethylene glycol, monoallyl ether, acetate

Inchi: InChI=1S/C9H16O4/c1-3-4-11-5-6-12-7-8-13-9(2)10/h3H,1,4-8H2,2H3
InchiKey: SIQNAPRKWIPLPE-UHFFFAOYSA-N
Formula: C9H16O4
SMILES: C=CCOCCOCCOC(C)=O
Mol. weight [g/mol]: 188.22

Physical Properties

Property code	Value	Unit	Source
gf	-331.18	kJ/mol	Joback Method
hf	-612.90	kJ/mol	Joback Method
hfus	22.95	kJ/mol	Joback Method
hvap	48.93	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.769		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1252.00		NIST Webbook
tb	523.13	K	Joback Method
tc	698.88	K	Joback Method
tf	306.05	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.45	J/mol×K	523.13	Joback Method
cpg	366.80	J/mol×K	552.42	Joback Method
cpg	378.75	J/mol×K	581.71	Joback Method
cpg	390.28	J/mol×K	611.00	Joback Method
cpg	401.39	J/mol×K	640.30	Joback Method
cpg	412.06	J/mol×K	669.59	Joback Method
cpg	422.29	J/mol×K	698.88	Joback Method
dvisc	0.0016686	Pa×s	306.05	Joback Method
dvisc	0.0009258	Pa×s	342.23	Joback Method
dvisc	0.0005750	Pa×s	378.41	Joback Method
dvisc	0.0003880	Pa×s	414.59	Joback Method
dvisc	0.0002789	Pa×s	450.77	Joback Method
dvisc	0.0002106	Pa×s	486.95	Joback Method
dvisc	0.0001653	Pa×s	523.13	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R151936&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

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