Diethylene glycol monoacetate

Other names: 2-(2-Hydroxyethoxy)ethyl acetate
Inchi: InChI=1S/C6H12O4/c1-6(8)10-5-4-9-3-2-7/h7H,2-5H2,1H3
InchiKey: XXXFZKQPYACQLD-UHFFFAOYSA-N
Formula: C6H12O4
SMILES: CC(=O)OCCOCCO
Mol. weight [g/mol]: 148.16
CAS: 2093-20-1

Physical Properties

Property code	Value	Unit	Source
gf	-476.10	kJ/mol	Joback Method
hf	-696.42	kJ/mol	Joback Method
hfus	19.36	kJ/mol	Joback Method
hvap	57.20	kJ/mol	Joback Method
log10ws	0.45		Crippen Method
logp	-0.442		Crippen Method
mcvol	114.580	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	1121.00		NIST Webbook
rinpol	1121.00		NIST Webbook
tb	527.57	K	Joback Method
tc	698.08	K	Joback Method
tf	312.59	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.46	J/mol×K	527.57	Joback Method
cpg	308.72	J/mol×K	669.66	Joback Method
cpg	301.06	J/mol×K	641.24	Joback Method
cpg	293.09	J/mol×K	612.82	Joback Method
cpg	284.83	J/mol×K	584.41	Joback Method
cpg	276.29	J/mol×K	555.99	Joback Method

cpg	316.08	J/mol×K	698.08	Joback Method
dvisc	0.0001175	Pa×s	527.57	Joback Method
dvisc	0.0001799	Pa×s	491.74	Joback Method
dvisc	0.0002945	Pa×s	455.91	Joback Method
dvisc	0.0005245	Pa×s	420.08	Joback Method
dvisc	0.0010404	Pa×s	384.25	Joback Method
dvisc	0.0023758	Pa×s	348.42	Joback Method
dvisc	0.0065558	Pa×s	312.59	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2093201&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

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