Diethoxymethyl acetate

Other names: Methanol, diethoxy-, acetate
Inchi: InChI=1S/C7H14O4/c1-4-9-7(10-5-2)11-6(3)8/h7H,4-5H2,1-3H3
InchiKey: IRUNKQSGDBYUDC-UHFFFAOYSA-N
Formula: C7H14O4
SMILES: CCOC(OCC)OC(C)=O
Mol. weight [g/mol]: 162.18
CAS: 14036-06-7

Physical Properties

Property code	Value	Unit	Source
gf	-438.30	kJ/mol	Joback Method
hf	-702.33	kJ/mol	Joback Method
hfus	15.53	kJ/mol	Joback Method
hvap	44.76	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	0.906		Crippen Method
mcvol	128.670	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	992.00		NIST Webbook
rinpol	992.00		NIST Webbook
tb	480.25	K	Joback Method
tc	659.47	K	Joback Method
tf	270.27	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.01	J/mol×K	480.25	Joback Method
cpg	296.18	J/mol×K	510.12	Joback Method
cpg	307.05	J/mol×K	539.99	Joback Method
cpg	317.61	J/mol×K	569.86	Joback Method
cpg	327.85	J/mol×K	599.73	Joback Method
cpg	337.74	J/mol×K	629.60	Joback Method

cpg	347.28	J/mol×K	659.47	Joback Method
dvisc	0.0024891	Pa×s	270.27	Joback Method
dvisc	0.0012521	Pa×s	305.27	Joback Method
dvisc	0.0007255	Pa×s	340.26	Joback Method
dvisc	0.0004654	Pa×s	375.26	Joback Method
dvisc	0.0003220	Pa×s	410.26	Joback Method
dvisc	0.0002361	Pa×s	445.25	Joback Method
dvisc	0.0001811	Pa×s	480.25	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=C14036067&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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