Acetic acid, diethoxy-, ethyl ester

Other names: Ethyl diethoxyacetate
Diethoxyacetic acid ethyl ester
Inchi: InChI=1S/C8H16O4/c1-4-10-7(9)8(11-5-2)12-6-3/h8H,4-6H2,1-3H3
InchiKey: XCLBIKIQSCTANZ-UHFFFAOYSA-N
Formula: C8H16O4
SMILES: CCOC(=O)C(OCC)OCC
Mol. weight [g/mol]: 176.21
CAS: 6065-82-3

Physical Properties

Property code	Value	Unit	Source
gf	-429.88	kJ/mol	Joback Method
hf	-722.97	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	46.99	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	0.949		Crippen Method
mcvol	142.760	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1092.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1487.00		NIST Webbook
tb	472.20	K	NIST Webbook
tc	680.70	K	Joback Method
tf	281.54	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.22	J/mol×K	503.13	Joback Method
cpg	340.49	J/mol×K	532.73	Joback Method
cpg	352.40	J/mol×K	562.32	Joback Method

cpg	363.94	J/mol×K	591.92	Joback Method
cpg	375.08	J/mol×K	621.51	Joback Method
cpg	385.82	J/mol×K	651.11	Joback Method
cpg	396.14	J/mol×K	680.70	Joback Method
dvisc	0.0024361	Pa×s	281.54	Joback Method
dvisc	0.0012025	Pa×s	318.47	Joback Method
dvisc	0.0006874	Pa×s	355.40	Joback Method
dvisc	0.0004366	Pa×s	392.34	Joback Method
dvisc	0.0002998	Pa×s	429.27	Joback Method
dvisc	0.0002185	Pa×s	466.20	Joback Method
dvisc	0.0001668	Pa×s	503.13	Joback Method

Sources

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=C6065823&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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