1,3-Diethoxypropane

Inchi: InChI=1S/C7H16O2/c1-3-8-6-5-7-9-4-2/h3-7H2,1-2H3
InchiKey: IOQSSIPMPIYMDF-UHFFFAOYSA-N
Formula: C7H16O2
SMILES: CCOCCCOCC
Mol. weight [g/mol]: 132.20
CAS: 3459-83-4

Physical Properties

Property code	Value	Unit	Source
chl	-4559.10 ± 1.40	kJ/mol	NIST Webbook
gf	-201.94	kJ/mol	Joback Method
hf	-436.20 ± 1.50	kJ/mol	NIST Webbook
hfl	-482.10 ± 1.50	kJ/mol	NIST Webbook
hfus	16.26	kJ/mol	Joback Method
hvap	45.92	kJ/mol	NIST Webbook
hvap	45.90 ± 0.20	kJ/mol	NIST Webbook
hvap	45.90 ± 0.20	kJ/mol	NIST Webbook
hvap	45.90	kJ/mol	NIST Webbook
log10ws	-0.93		Crippen Method
logp	1.450		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	828.20		NIST Webbook
rinpol	828.20		NIST Webbook
rinpol	836.50		NIST Webbook
tb	413.70	K	NIST Webbook
tc	569.26	K	Joback Method
tf	213.11	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.33	J/mol×K	404.40	Joback Method

cpg	253.59	J/mol×K	431.88	Joback Method
cpg	264.58	J/mol×K	459.35	Joback Method
cpg	275.28	J/mol×K	486.83	Joback Method
cpg	285.69	J/mol×K	514.30	Joback Method
cpg	295.82	J/mol×K	541.78	Joback Method
cpg	305.65	J/mol×K	569.26	Joback Method
dvisc	0.0029460	Pa×s	213.11	Joback Method
dvisc	0.0014040	Pa×s	244.99	Joback Method
dvisc	0.0007936	Pa×s	276.87	Joback Method
dvisc	0.0005047	Pa×s	308.75	Joback Method
dvisc	0.0003493	Pa×s	340.64	Joback Method
dvisc	0.0002575	Pa×s	372.52	Joback Method
dvisc	0.0001992	Pa×s	404.40	Joback Method
hvapt	37.17	kJ/mol	413.70	NIST Webbook

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=C3459834&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt: Enthalpy of vaporization at a given temperature
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