3,3-Diethoxy-1-propanol

Other names: 3,3-Diethoxypropanol
Inchi: InChI=1S/C7H16O3/c1-3-9-7(5-6-8)10-4-2/h7-8H,3-6H2,1-2H3
InchiKey: ASERXEZXVIJBRO-UHFFFAOYSA-N
Formula: C7H16O3
SMILES: CCOC(CCO)OCC
Mol. weight [g/mol]: 148.20
CAS: 16777-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-341.20	kJ/mol	Joback Method
hf	-609.76	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	52.29	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.768		Crippen Method
mcvol	127.100	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
ripol	1611.00		NIST Webbook
tb	496.14	K	Joback Method
tc	659.77	K	Joback Method
tf	258.93	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.11	J/mol×K	496.14	Joback Method
cpg	344.88	J/mol×K	632.50	Joback Method
cpg	335.57	J/mol×K	605.23	Joback Method
cpg	325.94	J/mol×K	577.96	Joback Method
cpg	315.98	J/mol×K	550.68	Joback Method
cpg	305.70	J/mol×K	523.41	Joback Method
cpg	353.86	J/mol×K	659.77	Joback Method

dvisc	0.0001127	Pa×s	496.14	Joback Method
dvisc	0.0001893	Pa×s	456.61	Joback Method
dvisc	0.0003507	Pa×s	417.07	Joback Method
dvisc	0.0007395	Pa×s	377.53	Joback Method
dvisc	0.0018565	Pa×s	338.00	Joback Method
dvisc	0.0059483	Pa×s	298.47	Joback Method
dvisc	0.0271956	Pa×s	258.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.70	K	1.90	NIST Webbook

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=C16777870&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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