3,3-Diethoxypropylamine

Other names: Propionaldehyde, 3-amino-, diethyl acetal
Inchi: InChI=1S/C7H17NO2/c1-3-9-7(5-6-8)10-4-2/h7H,3-6,8H2,1-2H3
InchiKey: PXXMSHBZYAOHBD-UHFFFAOYSA-N
Formula: C7H17NO2
SMILES: CCOC(CCN)OCC
Mol. weight [g/mol]: 147.22
CAS: 41365-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-137.93	kJ/mol	Joback Method
hf	-423.74	kJ/mol	Joback Method
hfus	17.94	kJ/mol	Joback Method
hvap	46.25	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.734		Crippen Method
mcvol	131.210	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
tb	476.49	K	Joback Method
tc	658.00	K	Joback Method
tf	281.37	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.96	J/mol×K	476.49	Joback Method
cpg	311.42	J/mol×K	506.74	Joback Method
cpg	323.48	J/mol×K	536.99	Joback Method
cpg	335.13	J/mol×K	567.25	Joback Method
cpg	346.36	J/mol×K	597.50	Joback Method
cpg	357.17	J/mol×K	627.75	Joback Method
cpg	367.55	J/mol×K	658.00	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=C41365757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume