

2-Ethylamino-2-methylpropane-1,3-diol, diethyl ether

Other names:	1,3-Diethoxy-N-ethyl-2-methylpropan-2-amine
Inchi:	InChI=1S/C10H23NO2/c1-5-11-10(4,8-12-6-2)9-13-7-3/h11H,5-9H2,1-4H3
InchiKey:	HTVSPMZEFGUELU-UHFFFAOYSA-N
Formula:	C10H23NO2
SMILES:	CCNC(C)(COCC)COCC
Mol. weight [g/mol]:	189.30

Physical Properties

Property code	Value	Unit	Source
gf	-84.45	kJ/mol	Joback Method
hf	-469.45	kJ/mol	Joback Method
hfus	21.72	kJ/mol	Joback Method
hvap	47.81	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.428		Crippen Method
mvol	173.480	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1115.00		NIST Webbook
tb	519.98	K	Joback Method
tc	694.91	K	Joback Method
tf	302.00	K	Joback Method
vc	0.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.54	J/molxK	519.98	Joback Method
cpg	441.40	J/molxK	549.14	Joback Method
cpg	456.61	J/molxK	578.29	Joback Method
cpg	471.18	J/molxK	607.45	Joback Method
cpg	485.11	J/molxK	636.60	Joback Method
cpg	498.42	J/molxK	665.76	Joback Method
cpg	511.13	J/molxK	694.91	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=U378722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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