

Diethylamine N-d1

Inchi:	InChI=1S/C4H11N/c1-3-5-4-2/h5H,3-4H2,1-2H3/i/hD
InchiKey:	HPNMFZURTQLUMO-DYCDLGHISA-N
Formula:	C4H10DN
SMILES:	CCNCC
Mol. weight [g/mol]:	74.14
CAS:	997-11-5

Physical Properties

Property code	Value	Unit	Source
gf	72.19	kJ/mol	Joback Method
hf	-72.42	kJ/mol	Joback Method
hfus	11.21	kJ/mol	Joback Method
hvap	30.93	kJ/mol	Joback Method
ie	8.31 ± 0.01	eV	NIST Webbook
log10ws	-0.69		Crippen Method
logp	0.616		Crippen Method
mcvol	77.200	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	341.09	K	Joback Method
tc	511.35	K	Joback Method
tf	187.50	K	Joback Method
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.62	J/mol×K	341.09	Joback Method
cpg	137.29	J/mol×K	369.47	Joback Method
cpg	145.65	J/mol×K	397.84	Joback Method
cpg	153.72	J/mol×K	426.22	Joback Method
cpg	161.49	J/mol×K	454.60	Joback Method
cpg	168.97	J/mol×K	482.97	Joback Method
cpg	176.17	J/mol×K	511.35	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=C997115&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
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
ie:	Ionization energy
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

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