2-(Diethylamino)acetonitrile

Other names:	Diethylaminoacetonitrile
	Acetonitrile, (diethylamino)-
	Glycinonitrile, N,N-diethyl-
	N,N-Diethylaminoacetonitrile
	Nitril kiseliny diethylaminooctove
Inchi:	InChI=1S/C6H12N2/c1-3-8(4-2)6-5-7/h3-4,6H2,1-2H3
InchiKey:	LVPZSMIBSMMLPI-UHFFFAOYSA-N
Formula:	C6H12N2
SMILES:	CCN(CC)CC#N
Mol. weight [g/mol]:	112.17
CAS:	3010-02-4

Physical Properties

Property code	Value	Unit	Source
chl	-4092.15 ± 0.85	kJ/mol	NIST Webbook
gf	243.60	kJ/mol	Joback Method
hf	66.00 ± 1.00	kJ/mol	NIST Webbook
hfl	16.10 ± 1.00	kJ/mol	NIST Webbook
hfus	15.82	kJ/mol	Joback Method
hvap	49.93 ± 0.27	kJ/mol	NIST Webbook
hvap	49.90	kJ/mol	NIST Webbook
log10ws	-0.77		Crippen Method
logp	0.852		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	912.00		NIST Webbook
tb	443.20	K	NIST Webbook
tc	638.03	K	Joback Method
tf	254.84	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	266.53	J/mol×K	606.89	Joback Method
cpg	219.32	J/mol×K	451.20	Joback Method
cpg	229.70	J/mol×K	482.34	Joback Method
cpg	239.60	J/mol×K	513.48	Joback Method
cpg	249.03	J/mol×K	544.61	Joback Method
cpg	258.00	J/mol×K	575.75	Joback Method
cpg	274.63	J/mol×K	638.03	Joback Method
hvapt	49.90 ± 0.30	kJ/mol	300.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.20	K	3.20	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C3010024&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume