Diethylcyanamide

Other names:	Cyanamide, diethyl- N,N-Diethylcyanamide USAF ek-6326 Diethylkyanamid
Inchi:	InChI=1S/C5H10N2/c1-3-7(4-2)5-6/h3-4H2,1-2H3
InchiKey:	ZZTSQZQUWBFTAT-UHFFFAOYSA-N
Formula:	C5H10N2
SMILES:	CCN(C#N)CC
Mol. weight [g/mol]:	98.15
CAS:	617-83-4

Physical Properties

Property code	Value	Unit	Source
chl	-3412.50 ± 1.80	kJ/mol	NIST Webbook
chl	-3412.50 ± 1.80	kJ/mol	NIST Webbook
gf	235.18	kJ/mol	Joback Method
hf	63.50	kJ/mol	NIST Webbook
hf	63.50 ± 2.10	kJ/mol	NIST Webbook
hf	63.50 ± 3.10	kJ/mol	NIST Webbook
hfl	15.80 ± 1.80	kJ/mol	NIST Webbook
hfl	15.80 ± 1.80	kJ/mol	NIST Webbook
hfus	13.23	kJ/mol	Joback Method
hvap	47.70	kJ/mol	NIST Webbook
hvap	47.70 ± 0.80	kJ/mol	NIST Webbook
hvap	47.70 ± 0.80	kJ/mol	NIST Webbook
ie	8.97	eV	NIST Webbook
log10ws	-0.85		Crippen Method
logp	0.809		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
tb	461.20	K	NIST Webbook
tc	616.90	K	Joback Method
tf	192.55 ± 0.20	K	NIST Webbook
tf	192.10 ± 0.35	K	NIST Webbook
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.63	J/mol×K	428.32	Joback Method
cpg	189.79	J/mol×K	459.75	Joback Method
cpg	198.52	J/mol×K	491.18	Joback Method
cpg	206.83	J/mol×K	522.61	Joback Method
cpg	214.74	J/mol×K	554.04	Joback Method
cpg	222.25	J/mol×K	585.47	Joback Method
cpg	229.39	J/mol×K	616.90	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C617834&Units=SI
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

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
ie: Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume