Propanenitrile, 3-(diethylamino)-

Other names:	Propionitrile, 3-(diethylamino)-
	N-(2-Cyanoethyl)diethylamine
	3-(Diethylamino)propionitrile
	3-(Diethylamino)propanenitrile
	3-diethylaminopropiononitrile
Inchi:	InChI=1S/C7H14N2/c1-3-9(4-2)7-5-6-8/h3-5,7H2,1-2H3
InchiKey:	LFFKXGFSDGRFQA-UHFFFAOYSA-N
Formula:	C7H14N2
SMILES:	CCN(CC)CCC#N
Mol. weight [g/mol]:	126.20
CAS:	5351-04-2

Physical Properties

Property code	Value	Unit	Source
gf	252.02	kJ/mol	Joback Method
hf	44.60	kJ/mol	Joback Method
hfus	18.41	kJ/mol	Joback Method
hvap	43.70	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.242		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	474.08	K	Joback Method
tc	659.05	K	Joback Method
tf	213.25 ± 0.30	K	NIST Webbook
tf	213.65 ± 0.20	K	NIST Webbook
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.38	J/mol×K	628.22	Joback Method
cpg	260.17	J/mol×K	474.08	Joback Method
cpg	271.65	J/mol×K	504.91	Joback Method

cpg	282.59	J/mol×K	535.74	Joback Method
cpg	293.01	J/mol×K	566.57	Joback Method
cpg	302.94	J/mol×K	597.39	Joback Method
cpg	321.36	J/mol×K	659.05	Joback Method
hvapt	53.70	kJ/mol	404.00	NIST Webbook

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=C5351042&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume