3-Dipropylaminopropanenitrile

Other names:	3-(Dipropylamino)propionitrile
	3-di-n-Propylaminopropionitrile
	Propanenitrile, 3-(dipropylamino)-
	3-(dipropylamino)propiononitrile
Inchi:	InChI=1S/C9H18N2/c1-3-7-11(8-4-2)9-5-6-10/h3-5,7-9H2,1-2H3
InchiKey:	TXKWRPYUNDNNMI-UHFFFAOYSA-N
Formula:	C9H18N2
SMILES:	CCCN(CCC)CCC#N
Mol. weight [g/mol]:	154.25
CAS:	20732-22-3

Physical Properties

Property code	Value	Unit	Source
gf	268.86	kJ/mol	Joback Method
hf	3.32	kJ/mol	Joback Method
hfus	23.59	kJ/mol	Joback Method
hvap	48.15	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.022		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
tb	519.84	K	Joback Method
tc	701.06	K	Joback Method
tf	288.65	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.90	J/mol×K	519.84	Joback Method
cpg	361.22	J/mol×K	550.04	Joback Method
cpg	373.92	J/mol×K	580.25	Joback Method
cpg	386.03	J/mol×K	610.45	Joback Method
cpg	397.56	J/mol×K	640.65	Joback Method

cpg	408.54	J/mol×K	670.85	Joback Method
cpg	418.99	J/mol×K	701.06	Joback Method

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=C20732223&Units=SI

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