

di-n-Propylaminoacetonitrile

Other names:	2-(Dipropylamino)acetonitrile Acetonitrile, (dipropylamino)- dipropylaminoacetonitrile
Inchi:	InChI=1S/C8H16N2/c1-3-6-10(7-4-2)8-5-9/h3-4,6-8H2,1-2H3
InchiKey:	ZFQYTSCUGODUDB-UHFFFAOYSA-N
Formula:	C8H16N2
SMILES:	CCCN(CC#N)CCC
Mol. weight [g/mol]:	140.23
CAS:	18071-35-7

Physical Properties

Property code	Value	Unit	Source
gf	260.44	kJ/mol	Joback Method
hf	23.96	kJ/mol	Joback Method
hfus	21.00	kJ/mol	Joback Method
hvap	45.92	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.632		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	496.96	K	Joback Method
tc	680.04	K	Joback Method
tf	277.38	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.07	J/molxK	496.96	Joback Method
cpg	315.52	J/molxK	527.47	Joback Method
cpg	327.39	J/molxK	557.99	Joback Method
cpg	338.71	J/molxK	588.50	Joback Method
cpg	349.48	J/molxK	619.01	Joback Method
cpg	359.74	J/molxK	649.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C18071357&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
mccvol:	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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