4-(Diethylamino)benzonitrile

Other names: p-Diethylaminobenzonitrile
Benzonitrile, 4-(diethylamino)-
Inchi: InChI=1S/C11H14N2/c1-3-13(4-2)11-7-5-10(9-12)6-8-11/h5-8H,3-4H2,1-2H3
InchiKey: KMLGFOAKCYHXCQ-UHFFFAOYSA-N
Formula: C11H14N2
SMILES: CCN(CC)c1ccc(C#N)cc1
Mol. weight [g/mol]: 174.24
CAS: 2873-90-7

Physical Properties

Property code	Value	Unit	Source
gf	388.48	kJ/mol	Joback Method
hf	187.10	kJ/mol	Joback Method
hfus	22.43	kJ/mol	Joback Method
hvap	55.54	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.404		Crippen Method
mcvol	153.450	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
tb	597.26	K	Joback Method
tc	814.24	K	Joback Method
tf	350.13	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.38	J/mol×K	597.26	Joback Method
cpg	383.04	J/mol×K	633.42	Joback Method
cpg	395.83	J/mol×K	669.59	Joback Method
cpg	407.79	J/mol×K	705.75	Joback Method
cpg	418.97	J/mol×K	741.91	Joback Method
cpg	429.41	J/mol×K	778.08	Joback Method
cpg	439.14	J/mol×K	814.24	Joback Method

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=C2873907&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
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