4-(Dicyanomethyl)nitrobenzene

Inchi: InChI=1S/C9H5N3O2/c10-5-8(6-11)7-1-3-9(4-2-7)12(13)14/h1-4,8H
InchiKey: HXEPLLFRQAVQQJ-UHFFFAOYSA-N
Formula: C9H5N3O2
SMILES: N#CC(C#N)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 187.15
CAS: 7077-65-8

Physical Properties

Property code	Value	Unit	Source
gf	427.15	kJ/mol	Joback Method
hf	309.69	kJ/mol	Joback Method
hfus	23.57	kJ/mol	Joback Method
hvap	75.73	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	1.726		Crippen Method
mcvol	134.090	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	792.54	K	Joback Method
tc	1059.17	K	Joback Method
tf	488.72	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.93	J/mol×K	792.54	Joback Method
cpg	340.41	J/mol×K	836.98	Joback Method
cpg	347.13	J/mol×K	881.42	Joback Method
cpg	353.16	J/mol×K	925.85	Joback Method
cpg	358.54	J/mol×K	970.29	Joback Method
cpg	363.34	J/mol×K	1014.73	Joback Method
cpg	367.60	J/mol×K	1059.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7077658&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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