1,2-Benzenediacetonitrile

Other names:	o-Benzenediacetonitrile
	o-Bis(cyanomethyl)benzene
	o-Xylylene dicyanide
	1,2-Phenylenediacetonitrile
	1,2-Bis(cyanomethyl)benzene
	o-Phenylenediacetonitrile
Inchi:	InChI=1S/C10H8N2/c11-7-5-9-3-1-2-4-10(9)6-8-12/h1-4H,5-6H2
InchiKey:	FWPFXBANOKKNBR-UHFFFAOYSA-N
Formula:	C10H8N2
SMILES:	N#CCc1ccccc1CC#N
Mol. weight [g/mol]:	156.18
CAS:	613-73-0

Physical Properties

Property code	Value	Unit	Source
gf	402.46	kJ/mol	Joback Method
hf	305.09	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	61.75	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.819		Crippen Method
mcvol	130.760	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	664.02	K	Joback Method
tc	902.09	K	Joback Method
tf	371.38	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.87	J/mol×K	664.02	Joback Method
cpg	314.46	J/mol×K	703.70	Joback Method
cpg	323.36	J/mol×K	743.38	Joback Method

cpg	331.60	J/mol×K	783.05	Joback Method
cpg	339.22	J/mol×K	822.73	Joback Method
cpg	346.26	J/mol×K	862.41	Joback Method
cpg	352.75	J/mol×K	902.09	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=C613730&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

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