1,3-Benzenediacetonitrile

Other names:	m-Benzenediacetonitrile m-Bis(cyanomethyl)benzene m-Phenylenediacetonitrile 1,3-Phenylenediacetonitrile 1,3-Bis(cyanomethyl)benzene m-Xylylene dicyanide Acetonitrile, m-phenylenedi- (3-Cyanomethyl-phenyl)-acetonitrile NSC 77095
Inchi:	InChI=1S/C10H8N2/c11-6-4-9-2-1-3-10(8-9)5-7-12/h1-3,8H,4-5H2
InchiKey:	GRPFZJNUYXIVSL-UHFFFAOYSA-N
Formula:	C10H8N2
SMILES:	N#CCc1cccc(CC#N)c1
Mol. weight [g/mol]:	156.18
CAS:	626-22-2

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	3.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626222&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

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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