1,3-Benzenedimethanamine

Other names:	m-Xylene-«alpha»,«alpha»'-diamine «alpha»,«alpha»'-m-Xylenediamine «alpha»,«alpha»'-Diamino-m-xylene m-Xylylenediamine 1,3-Bis(aminomethyl)benzene 1,3-Xylylenediamine m-Phenylenebis(methylamine) m-Xylylendiamin Methylamine, m-phenylenebis- MXDA 1,3-Bis-aminomethylbenzen NSC 61568 Epilink MX
Inchi:	InChI=1S/C8H12N2/c9-5-7-2-1-3-8(4-7)6-10/h1-4H,5-6,9-10H2
InchiKey:	FDLQZKYLHJJBHD-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	NCc1cccc(CN)c1
Mol. weight [g/mol]:	136.19
CAS:	1477-55-0

Physical Properties

Property code	Value	Unit	Source
gf	252.16	kJ/mol	Joback Method
hf	84.19	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	0.604		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1328.20		NIST Webbook
tb	520.20	K	NIST Webbook
tb	519.50 ± 1.50	K	NIST Webbook
tc	793.38	K	Joback Method
tf	385.38	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.99	J/mol×K	559.16	Joback Method
cpg	294.53	J/mol×K	598.20	Joback Method
cpg	306.24	J/mol×K	637.23	Joback Method
cpg	317.17	J/mol×K	676.27	Joback Method
cpg	327.34	J/mol×K	715.31	Joback Method
cpg	336.81	J/mol×K	754.34	Joback Method
cpg	345.59	J/mol×K	793.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	538.20	K	99.30	NIST Webbook
tbrp	413.00	K	1.90	NIST Webbook

Sources

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=C1477550&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume