

p-Xylylenediamine

Other names:	«alpha»,«alpha»'-Diamino-p-xylene 1,4-Benzenedimethanamine Methylamine, p-phenylenebis- 1,4-Bis-aminomethylbenzen 1,4-Bis(aminomethyl)benzene p-Phenylenebis(methylamine) p-Xylylendiamine 4-(Aminomethyl)benzylamine 1,4-Xylylenediamine p-Xylene-«alpha»,«alpha»'-diamine
Inchi:	InChI=1S/C8H12N2/c9-5-7-1-2-8(6-10)4-3-7/h1-4H,5-6,9-10H2
InchiKey:	ISKQADXMHQSTHK-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	NCc1ccc(CN)cc1
Mol. weight [g/mol]:	136.19
CAS:	539-48-0

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
tb	559.16	K	Joback Method
tc	793.38	K	Joback Method
tf	308.00	K	NIST Webbook
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	503.00	K	1.30	NIST Webbook

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=C539480&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
tbrp:	Boiling point at reduced pressure

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

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