3,3'-Diaminodiphenylmethane

Inchi: InChI=1S/C13H14N2/c14-12-5-1-3-10(8-12)7-11-4-2-6-13(15)9-11/h1-6,8-9H,7,14-15H2
InchiKey: CKOFBUUFHALZGK-UHFFFAOYSA-N
Formula: C13H14N2
SMILES: Nc1cccc(Cc2cccc(N)c2)c1
Mol. weight [g/mol]: 198.26
CAS: 19471-12-6

Physical Properties

Property code	Value	Unit	Source
gf	397.04	kJ/mol	Joback Method
hf	206.05	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	71.69	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.442		Crippen Method
mcvol	166.470	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	705.22	K	Joback Method
tc	964.17	K	Joback Method
tf	480.67	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.64	J/mol×K	705.22	Joback Method
cpg	456.08	J/mol×K	748.38	Joback Method
cpg	469.32	J/mol×K	791.54	Joback Method
cpg	481.43	J/mol×K	834.70	Joback Method
cpg	492.49	J/mol×K	877.85	Joback Method
cpg	502.58	J/mol×K	921.01	Joback Method
cpg	511.79	J/mol×K	964.17	Joback Method

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=C19471126&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume