

2,6-Dibromo-4-cyclohexylaniline

Inchi:	InChI=1S/C12H15Br2N/c13-10-6-9(7-11(14)12(10)15)8-4-2-1-3-5-8/h6-8H,1-5,15H2
InchiKey:	HWWWUEPYMLJAJK-UHFFFAOYSA-N
Formula:	C12H15Br2N
SMILES:	Nc1c(Br)cc(C2CCCCC2)cc1Br
Mol. weight [g/mol]:	333.06
CAS:	175135-11-2

Physical Properties

Property code	Value	Unit	Source
gf	253.22	kJ/mol	Joback Method
hf	51.88	kJ/mol	Joback Method
hfus	27.31	kJ/mol	Joback Method
hvap	70.51	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.841		Crippen Method
mcvol	190.300	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	739.98	K	Joback Method
tc	1014.63	K	Joback Method
tf	499.22	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.53	J/molxK	739.98	Joback Method
cpg	493.99	J/molxK	785.76	Joback Method
cpg	508.09	J/molxK	831.53	Joback Method
cpg	520.94	J/molxK	877.31	Joback Method
cpg	532.64	J/molxK	923.08	Joback Method
cpg	543.28	J/molxK	968.86	Joback Method
cpg	552.96	J/molxK	1014.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C175135112&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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