Benzenemethanamine, 2-amino-3,5-dibromo-N-cyclohexyl-N-methyl-

Other names: Toluene-«alpha»,2-diamine, 3,5-dibromo-N«alpha»-cyclohexyl-N«alpha»-methyl-
Bromexine
Bromhexine
Na 274
2-Amino-3,5-dibromo-N-cyclohexyl-N-methyl benzenemethanamine
2-Amino-3,5-dibromo-N-cyclohexyl-N-methylbenzenemathanamine

Inchi: InChI=1S/C14H20Br2N2/c1-18(12-5-3-2-4-6-12)9-10-7-11(15)8-13(16)14(10)17/h7-8,12H

InchiKey: OJGDCBLYJGHCIH-UHFFFAOYSA-N

Formula: C14H20Br2N2

SMILES: CN(Cc1cc(Br)cc(Br)c1N)C1CCCCC1

Mol. weight [g/mol]: 376.13

CAS: 3572-43-8

Physical Properties

Property code	Value	Unit	Source
gf	380.84	kJ/mol	Joback Method
hf	78.13	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method
hvap	77.00	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.558		Crippen Method
mcvol	228.460	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	2370.00		NIST Webbook
rinpol	2385.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2337.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
tb	798.18	K	Joback Method
tc	1055.32	K	Joback Method
tf	554.23	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.07	J/mol×K	798.18	Joback Method
cpg	642.17	J/mol×K	841.04	Joback Method
cpg	656.95	J/mol×K	883.89	Joback Method
cpg	670.50	J/mol×K	926.75	Joback Method
cpg	682.95	J/mol×K	969.61	Joback Method
cpg	694.40	J/mol×K	1012.46	Joback Method
cpg	704.97	J/mol×K	1055.32	Joback Method

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=C3572438&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume