Ambroxol

Other names:	Cyclohexanol, 4-[[(2-amino-3,5-dibromophenyl)methyl]amino]-, trans- Cyclohexanol, 4-((2-amino-3,5-dibromobenzyl)amino)- (E)- trans-4-((2-Amino-3,5-dibromobencil)amino)ciclohexanol trans-4-((2-Amino-3,5-dibromobenzyl)amino)cyclohexanol N-(trans-4-Hidroxiciclohexil)-(2-amino-3,5-dibromobencil)amina N-(trans-p-Hydroxycyclohexyl)-(2-amino-3,5-dibromobenzyl)amine N-(trans-4-Hydroxycyclohexyl)-(2-amino-3,5-dibromobenzyl)-amine NA-872 4-[(2-Amino-3,5-dibromobenzyl)amino]cyclohexanol, trans-
Inchi:	InChI=1S/C13H18Br2N2O/c14-9-5-8(13(16)12(15)6-9)7-17-10-1-3-11(18)4-2-10/h5-6,10-
InchiKey:	JBDGDEWWOUBZPM-UHFFFAOYSA-N
Formula:	C13H18Br2N2O
SMILES:	Nc1c(Br)cc(Br)cc1CNC1CCC(O)CC1
Mol. weight [g/mol]:	378.10
CAS:	18683-91-5

Physical Properties

Property code	Value	Unit	Source
gf	206.50	kJ/mol	Joback Method
hf	-87.86	kJ/mol	Joback Method
hfus	40.16	kJ/mol	Joback Method
hvap	95.54	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.187		Crippen Method
mcvol	220.240	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
tb	900.54	K	Joback Method
tc	1143.50	K	Joback Method
tf	619.73	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.72	J/mol×K	900.54	Joback Method
cpg	648.46	J/mol×K	941.03	Joback Method
cpg	659.19	J/mol×K	981.53	Joback Method
cpg	668.98	J/mol×K	1022.02	Joback Method
cpg	677.89	J/mol×K	1062.51	Joback Method
cpg	685.99	J/mol×K	1103.00	Joback Method
cpg	693.35	J/mol×K	1143.50	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18683915&Units=SI

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