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]: 378.11

Physical Properties

Property code	Value	Unit	Source
hfus	40.16	kJ/mol	Joback Method
logp	3.187		Crippen Method
mcvol	220.240	ml/mol	McGowan Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18683915&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices