

Urea, 1,1'-p-phenylenebis[3-(2-hydroxyethyl)-3-nitroso-

Inchi: InChI=1S/C12H16N6O6/c19-7-5-17(15-23)11(21)13-9-1-2-10(4-3-9)14-12(22)18(16-24)6
InchiKey: HMOWQMJSDDXBLW-UHFFFAOYSA-N
Formula: C12H16N6O6
SMILES: O=NN(CCO)C(=O)Nc1ccc(NC(=O)N(CCO)N=O)cc1
Mol. weight [g/mol]: 340.29
CAS: 116401-09-3

Physical Properties

Property code	Value	Unit	Source
hf	-689.95	kJ/mol	Joback Method
hvap	127.25	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	0.702		Crippen Method
mcvol	234.080	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	1049.74	K	Joback Method
tc	1289.30	K	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=C116401093&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

hf: Enthalpy of formation 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

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