

Hydroxyphenamate

Other names:

1,2-Butanediol, 2-phenyl-, 1-carbamate
«beta»-Ethyl-«beta»-hydroxyphenethyl carbamate
AI-0361
Listica
Oxyfenamate
Oxyphenamate
P 301
2-Hydroxy-2-Phenylbutyl carbamate
Carbamic acid, «beta»-ethyl-«beta»-hydroxyphenethyl ester
Hidroxifenamato
Phenylbutamate
Tensifen
2-Phenyl-1,2-butanediol 1-carbamate
«beta»-Ethyl-«beta»-hydroxyphenethyl carbamic acid ester
NSC-108034
Oxifenamate

Inchi:

InChI=1S/C11H15NO3/c1-2-11(14,8-15-10(12)13)9-6-4-3-5-7-9/h3-7,14H,2,8H2,1H3,(H2)

InchiKey:

WAFIYOULDIWAKR-UHFFFAOYSA-N

Formula:

C11H15NO3

SMILES:

CCC(O)(COC(=N)O)c1ccccc1

Mol. weight [g/mol]:

209.24

CAS:

50-19-1

Physical Properties

Property code	Value	Unit	Source
gf	-18.05	kJ/mol	Joback Method
hf	-280.94	kJ/mol	Joback Method
hvap	88.91	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	1.794		Crippen Method
mvol	165.380	ml/mol	McGowan Method
rinpol	1724.00		NIST Webbook
rinpol	1724.00		NIST Webbook
tb	765.65	K	Joback Method
tf	455.22	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.17	J/mol×K	765.65	Joback Method
cpg	61.88	J/mol×K	100.12	Joback Method
cpg	61.88	J/mol×K	100.12	Joback Method
cpg	61.88	J/mol×K	100.12	Joback Method
cpg	61.88	J/mol×K	100.12	Joback Method
cpg	61.88	J/mol×K	100.12	Joback Method
cpg	61.88	J/mol×K	100.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C50191&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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