

2H-1,3-oxazine-2-ethanol, 5,6-dihydro-b,b,5,5-tetramethyl-, carbanilate

Inchi:	InChI=1S/C17H24N2O3/c1-16(2)10-18-14(21-11-16)17(3,4)12-22-15(20)19-13-8-6-5-7-9
InchiKey:	HOUOBCVEXXPKS-UHFFFAOYSA-N
Formula:	C17H24N2O3
SMILES:	CC1(C)C=NC(C(C)(C)COC(=O)Nc2ccccc2)OC1
Mol. weight [g/mol]:	304.38
CAS:	96977-69-4

Physical Properties

Property code	Value	Unit	Source
gf	134.85	kJ/mol	Joback Method
hf	-311.79	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	79.99	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.715		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
tb	833.20	K	Joback Method
tc	1077.12	K	Joback Method
tf	560.92	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.93	J/molxK	833.20	Joback Method
cpg	812.01	J/molxK	873.85	Joback Method
cpg	830.08	J/molxK	914.51	Joback Method
cpg	847.34	J/molxK	955.16	Joback Method
cpg	863.97	J/molxK	995.82	Joback Method
cpg	880.14	J/molxK	1036.47	Joback Method
cpg	896.03	J/molxK	1077.12	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=C96977694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/114-873-6/2H-1-3-oxazine-2-ethanol-5-6-dihydro-b-b-5-5-tetramethyl-carbanilate.pdf>

Generated by Cheméo on 2024-05-01 19:57:35.191090112 +0000 UTC m=+16882704.111667438.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.