

Carbanilide, 2,2'-dimethyl-

Inchi: InChI=1S/C15H16N2O/c1-11-7-3-5-9-13(11)16-15(18)17-14-10-6-4-8-12(14)2/h3-10H,1-
InchiKey: WVYBLYKUAKXDLA-UHFFFAOYSA-N
Formula: C15H16N2O
SMILES: Cc1cccc1N=C(O)Nc1cccc1C
Mol. weight [g/mol]: 240.30
CAS: 617-07-2

Physical Properties

Property code	Value	Unit	Source
hf	70.86	kJ/mol	Joback Method
hvap	81.37	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.961		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
tb	824.83	K	Joback Method
tc	1056.88	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C617072&Units=SI>
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>

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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