

3-Anilinoacrylaldehyde anil

Inchi: InChI=1S/C15H14N2/c1-3-8-14(9-4-1)16-12-7-13-17-15-10-5-2-6-11-15/h1-13,16H/b12-7
InchiKey: ZFYNTCNECVPHDZ-RMPAWCBFSA-N
Formula: C15H14N2
SMILES: C(=CNc1ccccc1)C=Nc1ccccc1
Mol. weight [g/mol]: 222.29
CAS: 4485-89-6

Physical Properties

Property code	Value	Unit	Source
hf	373.04	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	4.015		Crippen Method
mcvol	186.050	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	726.97	K	Joback Method
tc	983.17	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4485896&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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