

Benzoic acid, 2-hydroximinoacetylamino-

Inchi:	InChI=1S/C9H8N2O4/c12-8(5-10-15)11-7-4-2-1-3-6(7)9(13)14/h1-5,15H,(H,11,12)(H,13,
InchiKey:	HKECZOKZNVYPQT-UHFFFAOYSA-N
Formula:	C9H8N2O4
SMILES:	O=C(C=NO)Nc1ccccc1C(=O)O
Mol. weight [g/mol]:	208.17
CAS:	6579-46-0

Physical Properties

Property code	Value	Unit	Source
hf	-397.96	kJ/mol	Joback Method
hvap	95.17	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.783		Crippen Method
mcvol	144.450	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	855.93	K	Joback Method
tc	1069.69	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C6579460&Units=SI

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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