

Naftazone

Inchi:	InChI=1S/C11H9N3O2/c12-11(16)14-13-9-6-5-7-3-1-2-4-8(7)10(9)15/h1-6H,(H3,12,14,16)
InchiKey:	TZGBBMBARSFJBG-UKTHLTGXSA-N
Formula:	C11H9N3O2
SMILES:	NC(=O)NN=C1C=Cc2ccccc2C1=O
Mol. weight [g/mol]:	215.21
CAS:	15687-37-3

Physical Properties

Property code	Value	Unit	Source
hf	-22.54	kJ/mol	Joback Method
hvap	75.92	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	0.920		Crippen Method
mcvol	155.710	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1448.00		NIST Webbook
tb	821.13	K	Joback Method
tc	1084.82	K	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=C15687373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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