

Benzoic acid, 4-(phenylazo)-

Other names:	Benzoic acid, p-(phenylazo)- p-Phenylazobenzoic acid Azobenzene-4-carboxylic acid Azoic acid 4-Carboxyazobenzene 4-phenylazobenzoic acid
Inchi:	InChI=1S/C13H10N2O2/c16-13(17)10-6-8-12(9-7-10)15-14-11-4-2-1-3-5-11/h1-9H,(H,16
InchiKey:	CSPTZWQFHBVOLO-UHFFFAOYSA-N
Formula:	C13H10N2O2
SMILES:	O=C(O)c1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]:	226.23
CAS:	1562-93-2

Physical Properties

Property code	Value	Unit	Source
hf	-67.65	kJ/mol	Joback Method
hvap	79.84	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.800		Crippen Method
mcvol	169.610	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
tb	850.43	K	Joback Method
tc	1096.31	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1562932&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

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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