

Benzoic acid, 4-hydroxy-3,5-dimethoxy-, hydrazide

Other names:	4-hydroxy-3,5-dimethoxybenzoic acid
Inchi:	InChI=1S/C9H12N2O4/c1-14-6-3-5(9(13)11-10)4-7(15-2)8(6)12/h3-4,12H,10H2,1-2H3,(H
InchiKey:	AKZAAANGIPRVDU-UHFFFAOYSA-N
Formula:	C9H12N2O4
SMILES:	COc1cc(C(=O)NN)cc(OC)c1O
Mol. weight [g/mol]:	212.20
CAS:	1443-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-219.65	kJ/mol	Joback Method
hf	-482.57	kJ/mol	Joback Method
hfus	32.38	kJ/mol	Joback Method
hvap	80.88	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	0.013		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
rinpol	1773.50		NIST Webbook
rinpol	1777.00		NIST Webbook
tb	743.99	K	Joback Method
tc	974.69	K	Joback Method
tf	584.68	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.57	J/molxK	743.99	Joback Method
cpg	432.91	J/molxK	782.44	Joback Method
cpg	442.60	J/molxK	820.89	Joback Method
cpg	451.69	J/molxK	859.34	Joback Method
cpg	460.21	J/molxK	897.79	Joback Method
cpg	468.19	J/molxK	936.24	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=C1443761&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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