Metacetamol

Other names:	3'-Hydroxyacetanilide
	3-(Acetylamino)-1-hydroxybenzene
	3-(Acetylamino)phenol
	3-acetamidophenol
	3-hydroxyacetanilide
	Acetamide, N-(3-hydroxyphenyl)-
	Acetanilide, 3'-hydroxy-
	BS 479
	BS 749
	Metalid
	N-(3-Hydroxyphenyl)acetamide
	N-Acetyl-m-Aminophenol
	NEBS
	NSC 3990
	Pedituss
	Pyrapap
	Rystal
	m-(Acetylamino)phenol
	m-Acetamidophenol
	m-Acetaminophenol
	m-hydroxyacetanilide
Inchi:	InChI=1S/C8H9NO2/c1-6(10)9-7-3-2-4-8(11)5-7/h2-5,11H,1H3,(H,9,10)
InchiKey:	QLNWXBAGRTUKKI-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	CC(=O)Nc1cccc(O)c1
Mol. weight [g/mol]:	151.16
CAS:	621-42-1

Physical Properties

Property code	Value	Unit	Source
gf	-65.26	kJ/mol	Joback Method
hf	-208.34	kJ/mol	Joback Method
hfus	23.00	kJ/mol	Joback Method
hvap	61.87	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.351		Crippen Method

mcvol	117.240	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	593.78	K	Joback Method
tc	827.84	K	Joback Method
tf	420.65	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.17	J/mol×K	593.78	Joback Method
cpg	290.67	J/mol×K	632.79	Joback Method
cpg	300.36	J/mol×K	671.80	Joback Method
cpg	309.33	J/mol×K	710.81	Joback Method
cpg	317.67	J/mol×K	749.82	Joback Method
cpg	325.46	J/mol×K	788.83	Joback Method
cpg	332.79	J/mol×K	827.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Partial molar volumes of some drug and pro-drug substances in 1-octanol at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2009.10.002
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=C621421&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume