4-Hydroxybenzamide

Other names: 4-Hydroxyphenylacetamide
Benzamide, 4-hydroxy-
p-Hydroxybenzamide
p-Hydroxyphenyl acetamide
Inchi: InChI=1S/C7H7NO2/c8-7(10)5-1-3-6(9)4-2-5/h1-4,9H,(H2,8,10)
InchiKey: QXSAKPUBHTZHKW-UHFFFAOYSA-N
Formula: C7H7NO2
SMILES: NC(=O)c1ccc(O)cc1
Mol. weight [g/mol]: 137.14
CAS: 619-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-96.62	kJ/mol	Joback Method
hf	-207.38	kJ/mol	Joback Method
hfus	25.20	kJ/mol	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
hvap	63.85	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	0.491		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	6009.25	kPa	Joback Method
tb	593.26	K	Joback Method
tc	841.84	K	Joback Method
tf	439.98	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.37	J/mol×K	593.26	Joback Method
cpg	251.48	J/mol×K	634.69	Joback Method
cpg	259.81	J/mol×K	676.12	Joback Method

cpg	267.46	J/mol×K	717.55	Joback Method
cpg	274.53	J/mol×K	758.98	Joback Method
cpg	281.13	J/mol×K	800.41	Joback Method
cpg	287.34	J/mol×K	841.84	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
Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study:	https://www.doi.org/10.1016/j.tca.2012.10.013
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=C619578&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