

(P-HYDROXYPHENYL)ACETAMIDE

Other names:	2-(4-Hydroxyphenyl)acetamide 2-(p-Hydroxyphenyl)acetamide 4-Hydroxybenzeneacetamide Acetamide, 2-(p-hydroxyphenyl)- Benzeneacetamide, 4-hydroxy- p-(Carbamoylmethyl)phenol p-Hydroxyphenylacetamide
Inchi:	InChI=1S/C8H9NO2/c9-8(11)5-6-1-3-7(10)4-2-6/h1-4,10H,5H2,(H2,9,11)
InchiKey:	YBPAYPRLUDCSEY-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	NC(=O)Cc1ccc(O)cc1
Mol. weight [g/mol]:	151.17

Physical Properties

Property code	Value	Unit	Source
hf	-316.13	kJ/mol	Cheméo Relay (1.0)
hfus	23.10	kJ/mol	Joback Method
hvap	78.04	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	Cheméo Relay (1.0)
log10ws	-2.39		Aqueous Solubility Prediction Method
logp	0.420		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
tb	568.06	K	Cheméo Relay (1.0)
tc	820.56	K	Cheméo Relay (1.0)
tf	416.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.26	J/mol×K	616.14	Joback Method
cpg	297.37	J/mol×K	656.67	Joback Method
cpg	306.69	J/mol×K	697.20	Joback Method
cpg	315.32	J/mol×K	737.73	Joback Method

cpg	323.34	J/mol×K	778.26	Joback Method
cpg	330.86	J/mol×K	818.79	Joback Method
cpg	337.98	J/mol×K	859.31	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17194820&Units=SI>

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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