Benzenepropanenitrile, «beta»-hydroxy-

Other names: Hydracrylonitrile, 3-phenyl-
Propionitrile, 3-hydroxy-3-phenyl-
3-Hydroxy-3-phenylpropanenitrile
Inchi: InChI=1S/C9H9NO/c10-7-6-9(11)8-4-2-1-3-5-8/h1-5,9,11H,6H2
InchiKey: HILDHWAXSORHRZ-UHFFFAOYSA-N
Formula: C9H9NO
SMILES: N#CCC(O)c1ccccc1
Mol. weight [g/mol]: 147.17
CAS: 17190-29-3

Physical Properties

Property code	Value	Unit	Source
gf	131.23	kJ/mol	Joback Method
hf	14.81	kJ/mol	Joback Method
hfus	15.18	kJ/mol	Joback Method
hvap	64.67	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.634		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	1431.40		NIST Webbook
rinpol	1431.40		NIST Webbook
tb	625.82	K	Joback Method
tc	840.17	K	Joback Method
tf	328.42	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.48	J/mol×K	625.82	Joback Method
cpg	297.98	J/mol×K	661.54	Joback Method
cpg	306.84	J/mol×K	697.27	Joback Method
cpg	315.09	J/mol×K	732.99	Joback Method

cpg	322.77	J/mol×K	768.72	Joback Method
cpg	329.90	J/mol×K	804.44	Joback Method
cpg	336.52	J/mol×K	840.17	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=C17190293&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