3,5-Dihydroxybenzonitrile

Other names: Benzonitrile, 3,5-dihydroxy-
Inchi: InChI=1S/C7H5NO2/c8-4-5-1-6(9)3-7(10)2-5/h1-3,9-10H
InchiKey: ABHOEQJNEOMTEK-UHFFFAOYSA-N
Formula: C7H5NO2
SMILES: N#Cc1cc(O)cc(O)c1
Mol. weight [g/mol]: 135.12
CAS: 19179-36-3

Physical Properties

Property code	Value	Unit	Source
gf	-55.59	kJ/mol	Joback Method
hf	-141.02	kJ/mol	Joback Method
hfus	21.00	kJ/mol	Joback Method
hvap	69.96	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	0.969		Crippen Method
mcvol	98.850	ml/mol	McGowan Method
pc	6046.69	kPa	Joback Method
tb	649.56	K	Joback Method
tc	907.13	K	Joback Method
tf	483.50	K	Joback Method
vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.38	J/mol×K	649.56	Joback Method
cpg	240.80	J/mol×K	692.49	Joback Method
cpg	246.75	J/mol×K	735.42	Joback Method
cpg	252.40	J/mol×K	778.34	Joback Method
cpg	257.92	J/mol×K	821.27	Joback Method
cpg	263.48	J/mol×K	864.20	Joback Method
cpg	269.25	J/mol×K	907.13	Joback Method

Sources

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=C19179363&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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