2-Hydroxy-3-methoxyphenylacetonitrile

Inchi: InChI=1S/C9H9NO2/c1-12-8-4-2-3-7(5-6-10)9(8)11/h2-4,11H,5H2,1H3
InchiKey: HGPGOFBJMBBPAX-UHFFFAOYSA-N
Formula: C9H9NO2
SMILES: COc1cccc(CC#N)c1O
Mol. weight [g/mol]: 163.17
CAS: 42973-56-8

Physical Properties

Property code	Value	Unit	Source
gf	1.24	kJ/mol	Joback Method
hf	-148.68	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	64.47	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.467		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	642.10	K	Joback Method
tc	877.45	K	Joback Method
tf	429.07	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.27	J/mol×K	642.10	Joback Method
cpg	317.99	J/mol×K	681.33	Joback Method
cpg	327.09	J/mol×K	720.55	Joback Method
cpg	335.63	J/mol×K	759.78	Joback Method
cpg	343.69	J/mol×K	799.00	Joback Method
cpg	351.31	J/mol×K	838.23	Joback Method
cpg	358.55	J/mol×K	877.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42973568&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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