3-Ethoxy-4-hydroxyphenylacetonitrile

Inchi: InChI=1S/C10H11NO2/c1-2-13-10-7-8(5-6-11)3-4-9(10)12/h3-4,7,12H,2,5H2,1H3
InchiKey: BGCWVBVMOUDBJE-UHFFFAOYSA-N
Formula: C10H11NO2
SMILES: CCOc1cc(CC#N)ccc1O
Mol. weight [g/mol]: 177.20
CAS: 205748-01-2

Physical Properties

Property code	Value	Unit	Source
gf	9.66	kJ/mol	Joback Method
hf	-169.32	kJ/mol	Joback Method
hfus	23.79	kJ/mol	Joback Method
hvap	66.69	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.857		Crippen Method
mcvol	141.120	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
tb	664.98	K	Joback Method
tc	895.67	K	Joback Method
tf	440.34	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.73	J/mol×K	664.98	Joback Method
cpg	366.33	J/mol×K	703.43	Joback Method
cpg	376.29	J/mol×K	741.88	Joback Method
cpg	385.66	J/mol×K	780.32	Joback Method
cpg	394.51	J/mol×K	818.77	Joback Method
cpg	402.91	J/mol×K	857.22	Joback Method
cpg	410.90	J/mol×K	895.67	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C205748012&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