2-Ethoxyphenylacetonitrile

Inchi: InChI=1S/C10H11NO/c1-2-12-10-6-4-3-5-9(10)7-8-11/h3-6H,2,7H2,1H3
InchiKey: XXLCVIZGVFWXFL-UHFFFAOYSA-N
Formula: C10H11NO
SMILES: CCOc1ccccc1CC#N
Mol. weight [g/mol]: 161.20
CAS: 74205-51-9

Physical Properties

Property code	Value	Unit	Source
gf	164.28	kJ/mol	Joback Method
hf	7.99	kJ/mol	Joback Method
hfus	18.00	kJ/mol	Joback Method
hvap	53.68	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.151		Crippen Method
mcvol	135.250	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	584.36	K	Joback Method
tc	805.88	K	Joback Method
tf	328.62	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.69	J/mol×K	584.36	Joback Method
cpg	322.72	J/mol×K	621.28	Joback Method
cpg	334.06	J/mol×K	658.20	Joback Method
cpg	344.72	J/mol×K	695.12	Joback Method
cpg	354.71	J/mol×K	732.04	Joback Method
cpg	364.05	J/mol×K	768.96	Joback Method
cpg	372.76	J/mol×K	805.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74205519&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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