4-Ethylphenylacetonitrile

Inchi: InChI=1S/C10H11N/c1-2-9-3-5-10(6-4-9)7-8-11/h3-6H,2,7H2,1H3
InchiKey: NCPKDFDQDZMXCO-UHFFFAOYSA-N
Formula: C10H11N
SMILES: CCc1ccc(CC#N)cc1
Mol. weight [g/mol]: 145.20
CAS: 51632-28-1

Physical Properties

Property code	Value	Unit	Source
gf	269.28	kJ/mol	Joback Method
hf	140.21	kJ/mol	Joback Method
hfus	16.81	kJ/mol	Joback Method
hvap	51.27	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.315		Crippen Method
mcvol	129.380	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
tb	561.94	K	Joback Method
tc	786.30	K	Joback Method
tf	306.39	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.73	J/mol×K	561.94	Joback Method
cpg	299.96	J/mol×K	599.33	Joback Method
cpg	311.43	J/mol×K	636.73	Joback Method
cpg	322.18	J/mol×K	674.12	Joback Method
cpg	332.25	J/mol×K	711.51	Joback Method
cpg	341.65	J/mol×K	748.91	Joback Method
cpg	350.43	J/mol×K	786.30	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=C51632281&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