4-Isopropylphenylacetonitrile

Inchi: InChI=1S/C11H13N/c1-9(2)11-5-3-10(4-6-11)7-8-12/h3-6,9H,7H2,1-2H3
InchiKey: RIPHZOPMCRSGSI-UHFFFAOYSA-N
Formula: C11H13N
SMILES: CC(C)c1ccc(CC#N)cc1
Mol. weight [g/mol]: 159.23
CAS: 4395-87-3

Physical Properties

Property code	Value	Unit	Source
gf	275.26	kJ/mol	Joback Method
hf	114.29	kJ/mol	Joback Method
hfus	15.88	kJ/mol	Joback Method
hvap	53.11	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.876		Crippen Method
mcvol	143.470	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	584.38	K	Joback Method
tc	809.46	K	Joback Method
tf	302.66	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.15	J/mol×K	584.38	Joback Method
cpg	347.60	J/mol×K	621.89	Joback Method
cpg	360.22	J/mol×K	659.41	Joback Method
cpg	372.02	J/mol×K	696.92	Joback Method
cpg	383.06	J/mol×K	734.43	Joback Method
cpg	393.36	J/mol×K	771.94	Joback Method
cpg	402.97	J/mol×K	809.46	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=C4395873&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