4-Iodophenylacetonitrile

Inchi: InChI=1S/C8H6IN/c9-8-3-1-7(2-4-8)5-6-10/h1-4H,5H2
InchiKey: PNXWQTYSBFGIFD-UHFFFAOYSA-N
Formula: C8H6IN
SMILES: N#CCc1ccc(I)cc1
Mol. weight [g/mol]: 243.04
CAS: 51628-12-7

Physical Properties

Property code	Value	Unit	Source
gf	310.56	kJ/mol	Joback Method
hf	258.36	kJ/mol	Joback Method
hfus	16.04	kJ/mol	Joback Method
hvap	56.19	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.357		Crippen Method
mcvol	127.020	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	609.32	K	Joback Method
tc	873.92	K	Joback Method
tf	341.91	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.40	J/mol×K	609.32	Joback Method
cpg	247.34	J/mol×K	653.42	Joback Method
cpg	255.52	J/mol×K	697.52	Joback Method
cpg	263.01	J/mol×K	741.62	Joback Method
cpg	269.87	J/mol×K	785.72	Joback Method
cpg	276.15	J/mol×K	829.82	Joback Method
cpg	281.92	J/mol×K	873.92	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=C51628127&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