Iodoacetonitrile

Other names: Acetonitrile, iodo-
Inchi: InChI=1S/C2H2IN/c3-1-2-4/h1H2
InchiKey: VODKOOOHHCAWFR-UHFFFAOYSA-N
Formula: C2H2IN
SMILES: N#CCI
Mol. weight [g/mol]: 166.95
CAS: 624-75-9

Physical Properties

Property code	Value	Unit	Source
gf	157.26	kJ/mol	Joback Method
hf	157.14	kJ/mol	Joback Method
hfus	6.85	kJ/mol	Joback Method
hvap	39.90	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	0.945		Crippen Method
mcvol	66.240	ml/mol	McGowan Method
pc	4710.65	kPa	Joback Method
tb	440.38	K	Joback Method
tc	676.47	K	Joback Method
tf	235.35	K	Joback Method
vc	0.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	81.26	J/mol×K	440.38	Joback Method
cpg	84.10	J/mol×K	479.73	Joback Method
cpg	86.74	J/mol×K	519.08	Joback Method
cpg	89.18	J/mol×K	558.43	Joback Method
cpg	91.43	J/mol×K	597.78	Joback Method
cpg	93.53	J/mol×K	637.12	Joback Method
cpg	95.48	J/mol×K	676.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	456.20	K	96.00	NIST Webbook

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=C624759&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume