1-Fluoro-3-iodo-5-nitrobenzene

Other names: Benzene, 1-fluoro-3-iodo-5-nitro-
3-Fluoro-5-iodonitrobenzene
Inchi: InChI=1S/C6H3FINO2/c7-4-1-5(8)3-6(2-4)9(10)11/h1-3H
InchiKey: MXPYCSFCKXSPAB-UHFFFAOYSA-N
Formula: C6H3FINO2
SMILES: O=[N+]([O-])c1cc(F)cc(I)c1
Mol. weight [g/mol]: 267.00
CAS: 3819-88-3

Physical Properties

Property code	Value	Unit	Source
gf	-8.35	kJ/mol	Joback Method
hf	-83.58	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	57.70	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.338		Crippen Method
mcvol	116.650	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	617.57	K	Joback Method
tc	892.55	K	Joback Method
tf	411.10	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.74	J/mol×K	617.57	Joback Method
cpg	228.49	J/mol×K	663.40	Joback Method
cpg	235.51	J/mol×K	709.23	Joback Method
cpg	241.85	J/mol×K	755.06	Joback Method
cpg	247.58	J/mol×K	800.89	Joback Method
cpg	252.75	J/mol×K	846.72	Joback Method
cpg	257.42	J/mol×K	892.55	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=C3819883&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