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

Physical Properties

Property code	Value	Unit	Source
hfus	23.41	kJ/mol	Joback Method
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	-3.69		Cheméo Relay (1.0)
logp	2.339		Crippen Method
mcvol	116.650	ml/mol	McGowan Method
tb	532.60	K	Cheméo Relay (1.0)
tf	338.47	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3819883&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point