2,4-DIFLUORO-1-NITROBENZENE

Other names: 1,3-Difluoro-4-nitrobenzene
1-Nitro-2,4-difluorobenzene
2,4-Difluoro-1-nitrobenzene
Benzene, 2,4-difluoro-1-nitro-
Inchi: InChI=1S/C6H3F2NO2/c7-4-1-2-6(9(10)11)5(8)3-4/h1-3H
InchiKey: RJXOVESYJFXCGI-UHFFFAOYSA-N
Formula: C6H3F2NO2
SMILES: O=[N+]([O-])c1ccc(F)cc1F
Mol. weight [g/mol]: 159.09

Physical Properties

Property code	Value	Unit	Source
hfus	22.08	kJ/mol	Joback Method
ie	9.97	eV	Cheméo Relay (1.0)
log10ws	-2.73		Cheméo Relay (1.0)
logp	1.873		Crippen Method
mcvol	92.600	ml/mol	McGowan Method
tb	476.70	K	NIST Webbook
tb	476.50 ± 0.50	K	NIST Webbook
tb	480.20	K	NIST Webbook
tf	306.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.39	J/mol×K	523.70	Joback Method
cpg	203.84	J/mol×K	562.02	Joback Method
cpg	211.70	J/mol×K	600.33	Joback Method
cpg	219.01	J/mol×K	638.65	Joback Method
cpg	225.78	J/mol×K	676.96	Joback Method
cpg	232.03	J/mol×K	715.28	Joback Method
cpg	237.80	J/mol×K	753.60	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C446355&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