2,6-Difluoro-3-methylbenzoic acid, 2-nitro-5-fluorophenyl ester

Inchi: InChI=1S/C14H8F3NO4/c1-7-2-4-9(16)12(13(7)17)14(19)22-11-6-8(15)3-5-10(11)18(20)
InchiKey: QCJJZJLJSOZVNE-UHFFFAOYSA-N
Formula: C14H8F3NO4
SMILES: Cc1ccc(F)c(C(=O)Oc2cc(F)ccc2[N+](=O)[O-])c1F
Mol. weight [g/mol]: 311.21

Physical Properties

Property code	Value	Unit	Source
gf	-539.13	kJ/mol	Joback Method
hf	-760.47	kJ/mol	Joback Method
hfus	41.54	kJ/mol	Joback Method
hvap	77.92	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	3.540		Crippen Method
mcvol	190.770	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	2109.00		NIST Webbook
rinpol	2109.00		NIST Webbook
tb	823.92	K	Joback Method
tc	1058.23	K	Joback Method
tf	580.52	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.53	J/mol×K	823.92	Joback Method
cpg	536.60	J/mol×K	862.97	Joback Method
cpg	545.69	J/mol×K	902.02	Joback Method
cpg	553.82	J/mol×K	941.07	Joback Method
cpg	561.01	J/mol×K	980.12	Joback Method
cpg	567.27	J/mol×K	1019.18	Joback Method
cpg	572.64	J/mol×K	1058.23	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=U357685&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume