2,5-Difluorobenzoic acid, 2-nitro-5-fluorophenyl ester

Inchi: InChI=1S/C13H6F3NO4/c14-7-1-3-10(16)9(5-7)13(18)21-12-6-8(15)2-4-11(12)17(19)20/h

InchiKey: TXOSMCODEHGHPJ-UHFFFAOYSA-N

Formula: C13H6F3NO4

SMILES: O=C(Oc1cc(F)ccc1[N+](=O)[O-])c1cc(F)ccc1F

Mol. weight [g/mol]: 297.19

Physical Properties

Property code	Value	Unit	Source
gf	-537.92	kJ/mol	Joback Method
hf	-728.36	kJ/mol	Joback Method
hfus	39.34	kJ/mol	Joback Method
hvap	75.03	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.231		Crippen Method
mcvol	176.680	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1958.00		NIST Webbook
rinpol	1958.00		NIST Webbook
tb	796.06	K	Joback Method
tc	1033.47	K	Joback Method
tf	556.73	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.61	J/mol×K	796.06	Joback Method
cpg	485.34	J/mol×K	835.63	Joback Method
cpg	494.10	J/mol×K	875.20	Joback Method
cpg	501.94	J/mol×K	914.76	Joback Method
cpg	508.86	J/mol×K	954.33	Joback Method
cpg	514.91	J/mol×K	993.90	Joback Method
cpg	520.09	J/mol×K	1033.47	Joback Method

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=U357583&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume