2,5-Difluorobenzoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C13H7F2NO4/c14-8-1-6-12(15)11(7-8)13(17)20-10-4-2-9(3-5-10)16(18)19/h1-
InchiKey: AVQKHGLGGQZWJR-UHFFFAOYSA-N
Formula: C13H7F2NO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1cc(F)ccc1F
Mol. weight [g/mol]: 279.20

Physical Properties

Property code	Value	Unit	Source
gf	-333.48	kJ/mol	Joback Method
hf	-520.78	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	75.18	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.092		Crippen Method
mcvol	174.910	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	2118.00		NIST Webbook
tb	791.81	K	Joback Method
tc	1038.35	K	Joback Method
tf	543.62	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.72	J/mol×K	791.81	Joback Method
cpg	480.06	J/mol×K	832.90	Joback Method
cpg	489.35	J/mol×K	873.99	Joback Method
cpg	497.64	J/mol×K	915.08	Joback Method
cpg	504.96	J/mol×K	956.17	Joback Method
cpg	511.34	J/mol×K	997.26	Joback Method
cpg	516.82	J/mol×K	1038.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357586&Units=SI
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

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