2,6-Difluoro-3-methylbenzoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C14H9F2NO4/c1-8-2-7-11(15)12(13(8)16)14(18)21-10-5-3-9(4-6-10)17(19)20/
InchiKey: LLQAGHNZYQXOCB-UHFFFAOYSA-N
Formula: C14H9F2NO4
SMILES: Cc1ccc(F)c(C(=O)Oc2ccc([N+](=O)[O-])cc2)c1F
Mol. weight [g/mol]: 293.22

Physical Properties

Property code	Value	Unit	Source
gf	-334.69	kJ/mol	Joback Method
hf	-552.89	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	78.07	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	3.401		Crippen Method
mcvol	189.000	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	2227.00		NIST Webbook
tb	819.67	K	Joback Method
tc	1062.35	K	Joback Method
tf	567.41	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.68	J/mol×K	819.67	Joback Method
cpg	531.35	J/mol×K	860.12	Joback Method
cpg	540.96	J/mol×K	900.56	Joback Method
cpg	549.54	J/mol×K	941.01	Joback Method
cpg	557.13	J/mol×K	981.45	Joback Method
cpg	563.75	J/mol×K	1021.90	Joback Method
cpg	569.43	J/mol×K	1062.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357687&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

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