3-Fluorobenzoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C13H8FNO4/c14-10-3-1-2-9(8-10)13(16)19-12-6-4-11(5-7-12)15(17)18/h1-8H
InchiKey: SUBDOSZYYCCUGC-UHFFFAOYSA-N
Formula: C13H8FNO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1cccc(F)c1
Mol. weight [g/mol]: 261.21

Physical Properties

Property code	Value	Unit	Source
gf	-129.04	kJ/mol	Joback Method
hf	-313.20	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	75.34	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	2.953		Crippen Method
mcvol	173.140	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	787.56	K	Joback Method
tc	1044.15	K	Joback Method
tf	530.51	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.79	J/mol×K	787.56	Joback Method
cpg	474.79	J/mol×K	830.33	Joback Method
cpg	484.66	J/mol×K	873.09	Joback Method
cpg	493.43	J/mol×K	915.86	Joback Method
cpg	501.16	J/mol×K	958.62	Joback Method
cpg	507.90	J/mol×K	1001.39	Joback Method
cpg	513.70	J/mol×K	1044.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307730&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