3-Fluoro-5-trifluoromethylbenzoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C14H7F4NO4/c15-10-6-8(5-9(7-10)14(16,17)18)13(20)23-12-3-1-11(2-4-12)19

InchiKey: QTLNOZSGHDQFBP-UHFFFAOYSA-N

Formula: C14H7F4NO4

SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 329.20

Physical Properties

Property code	Value	Unit	Source
gf	-711.84	kJ/mol	Joback Method
hf	-942.39	kJ/mol	Joback Method
hfus	37.98	kJ/mol	Joback Method
hvap	74.48	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	3.972		Crippen Method
mcvol	192.540	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	810.00	K	Joback Method
tc	1044.90	K	Joback Method
tf	558.49	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.75	J/mol×K	810.00	Joback Method
cpg	549.60	J/mol×K	849.15	Joback Method
cpg	558.47	J/mol×K	888.30	Joback Method
cpg	566.42	J/mol×K	927.45	Joback Method
cpg	573.51	J/mol×K	966.60	Joback Method
cpg	579.81	J/mol×K	1005.75	Joback Method
cpg	585.39	J/mol×K	1044.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357963&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