3-Fluoro-4-trifluoromethylbenzoic acid, 2-nitro-5-fluorophenyl ester

Inchi: InChI=1S/C14H6F5NO4/c15-8-2-4-11(20(22)23)12(6-8)24-13(21)7-1-3-9(10(16)5-7)14(1

InchiKey: DAPFEKYCBRFPJK-UHFFFAOYSA-N

Formula: C14H6F5NO4

SMILES: O=C(Oc1cc(F)ccc1[N+](=O)[O-])c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 347.19

Physical Properties

Property code	Value	Unit	Source
gf	-916.28	kJ/mol	Joback Method
hf	-1149.97	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.111		Crippen Method
mcvol	194.310	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1916.00		NIST Webbook
rinpol	1916.00		NIST Webbook
tb	814.25	K	Joback Method
tc	1041.36	K	Joback Method
tf	571.60	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.57	J/mol×K	814.25	Joback Method
cpg	554.88	J/mol×K	852.10	Joback Method
cpg	563.27	J/mol×K	889.95	Joback Method
cpg	570.79	J/mol×K	927.80	Joback Method
cpg	577.52	J/mol×K	965.66	Joback Method
cpg	583.48	J/mol×K	1003.51	Joback Method
cpg	588.75	J/mol×K	1041.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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