

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

Inchi:	InChI=1S/C14H6F5NO4/c15-7-4-5-10(20(22)23)11(6-7)24-13(21)8-2-1-3-9(12(8)16)14(1
InchiKey:	KOICMPRNQPBZSO-UHFFFAOYSA-N
Formula:	C14H6F5NO4
SMILES:	O=C(Oc1cc(F)ccc1[N+](=O)[O-])c1cccc(C(F)(F)F)c1F
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	1954.00		NIST Webbook
rinpol	1954.00		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/molxK	814.25	Joback Method
cpg	554.88	J/molxK	852.10	Joback Method
cpg	563.27	J/molxK	889.95	Joback Method
cpg	570.79	J/molxK	927.80	Joback Method
cpg	577.52	J/molxK	965.66	Joback Method
cpg	583.48	J/molxK	1003.51	Joback Method
cpg	588.75	J/molxK	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=U357650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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