

4-Fluoro-2-trifluoromethylbenzoic acid, 4-nitrophenyl ester

Inchi:	InChI=1S/C14H7F4NO4/c15-8-1-6-11(12(7-8)14(16,17)18)13(20)23-10-4-2-9(3-5-10)19(
InchiKey:	KUWCCYCHUZGBOP-UHFFFAOYSA-N
Formula:	C14H7F4NO4
SMILES:	O=C(Oc1ccc([N+](=O)[O-])cc1)c1ccc(F)cc1C(F)(F)F
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	2041.00		NIST Webbook
rinpol	2041.00		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/molxK	810.00	Joback Method
cpg	549.60	J/molxK	849.15	Joback Method
cpg	558.47	J/molxK	888.30	Joback Method
cpg	566.42	J/molxK	927.45	Joback Method
cpg	573.51	J/molxK	966.60	Joback Method
cpg	579.81	J/molxK	1005.75	Joback Method
cpg	585.39	J/molxK	1044.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U357671&Units=SI

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

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