

3-Fluoro-5-trifluoromethylbenzoic acid, phenyl ester

Inchi:	InChI=1S/C14H8F4O2/c15-11-7-9(6-10(8-11)14(16,17)18)13(19)20-12-4-2-1-3-5-12/h1-8
InchiKey:	BQMZNYOYJDZWOD-UHFFFAOYSA-N
Formula:	C14H8F4O2
SMILES:	O=C(Oc1ccccc1)c1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	284.21

Physical Properties

Property code	Value	Unit	Source
gf	-737.76	kJ/mol	Joback Method
hf	-920.16	kJ/mol	Joback Method
hfus	27.01	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.064		Crippen Method
mcvol	175.120	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook
tb	653.18	K	Joback Method
tc	868.14	K	Joback Method
tf	402.36	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.52	J/molxK	653.18	Joback Method
cpg	462.17	J/molxK	689.01	Joback Method
cpg	473.82	J/molxK	724.83	Joback Method
cpg	484.53	J/molxK	760.66	Joback Method
cpg	494.35	J/molxK	796.49	Joback Method
cpg	503.33	J/molxK	832.31	Joback Method
cpg	511.53	J/molxK	868.14	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=U357955&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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