

2-Fluoro-5-trifluoromethylbenzoic acid, pentyl ester

Inchi:	InChI=1S/C13H14F4O2/c1-2-3-4-7-19-12(18)10-8-9(13(15,16)17)5-6-11(10)14/h5-6,8H,2
InchiKey:	AILLPNOUEPVZOQ-UHFFFAOYSA-N
Formula:	C13H14F4O2
SMILES:	CCCCCOC(=O)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]:	278.24

Physical Properties

Property code	Value	Unit	Source
gf	-858.59	kJ/mol	Joback Method
hf	-1136.05	kJ/mol	Joback Method
hfus	30.38	kJ/mol	Joback Method
hvap	52.72	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.192		Crippen Method
mcvol	184.790	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
tb	603.62	K	Joback Method
tc	785.28	K	Joback Method
tf	364.67	K	Joback Method
vc	0.741	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.37	J/mol×K	603.62	Joback Method
cpg	491.78	J/mol×K	633.90	Joback Method
cpg	504.45	J/mol×K	664.17	Joback Method
cpg	516.41	J/mol×K	694.45	Joback Method
cpg	527.67	J/mol×K	724.73	Joback Method
cpg	538.27	J/mol×K	755.00	Joback Method
cpg	548.24	J/mol×K	785.28	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=U338958&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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