

3-Fluoro-4-trifluoromethylbenzoic acid, 3-methylbutyl ester

Inchi:	InChI=1S/C13H14F4O2/c1-8(2)5-6-19-12(18)9-3-4-10(11(14)7-9)13(15,16)17/h3-4,7-8H,
InchiKey:	MQAVINCZLSZCPQ-UHFFFAOYSA-N
Formula:	C13H14F4O2
SMILES:	CC(C)CCOC(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]:	278.24

Physical Properties

Property code	Value	Unit	Source
gf	-861.03	kJ/mol	Joback Method
hf	-1141.33	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	52.34	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.047		Crippen Method
mcvol	184.790	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook
tb	603.18	K	Joback Method
tc	788.04	K	Joback Method
tf	349.67	K	Joback Method
vc	0.735	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.78	J/molxK	603.18	Joback Method
cpg	492.48	J/molxK	633.99	Joback Method
cpg	505.40	J/molxK	664.80	Joback Method
cpg	517.57	J/molxK	695.61	Joback Method
cpg	529.02	J/molxK	726.42	Joback Method
cpg	539.78	J/molxK	757.23	Joback Method
cpg	549.87	J/molxK	788.04	Joback Method

Sources

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=U360593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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