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

Inchi: InChI=1S/C11H10F4O3/c1-17-4-5-18-10(16)8-3-2-7(12)6-9(8)11(13,14)15/h2-3,6H,4-5H

InchiKey: SUNWGNSZMSDICB-UHFFFAOYSA-N

Formula: C11H10F4O3

SMILES: COCCOC(=O)c1ccc(F)cc1C(F)(F)F

Mol. weight [g/mol]: 266.19

Physical Properties

Property code	Value	Unit	Source
gf	-980.43	kJ/mol	Joback Method
hf	-1226.99	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.648		Crippen Method
mcvol	162.480	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1335.00		NIST Webbook
rinpol	1335.00		NIST Webbook
tb	580.28	K	Joback Method
tc	764.52	K	Joback Method
tf	364.36	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.55	J/mol×K	580.28	Joback Method
cpg	418.44	J/mol×K	610.99	Joback Method
cpg	429.69	J/mol×K	641.69	Joback Method
cpg	440.32	J/mol×K	672.40	Joback Method
cpg	450.33	J/mol×K	703.11	Joback Method
cpg	459.74	J/mol×K	733.81	Joback Method
cpg	468.56	J/mol×K	764.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343765&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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