3-Fluoro-4-trifluoromethylbenzoic acid, 2-ethoxyethyl ester

Inchi: InChI=1S/C12H12F4O3/c1-2-18-5-6-19-11(17)8-3-4-9(10(13)7-8)12(14,15)16/h3-4,7H,2,
InchiKey: FYWUAFJCEREHBU-UHFFFAOYSA-N
Formula: C12H12F4O3
SMILES: CCOCCOC(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 280.22

Physical Properties

Property code	Value	Unit	Source
gf	-972.01	kJ/mol	Joback Method
hf	-1247.63	kJ/mol	Joback Method
hfus	28.98	kJ/mol	Joback Method
hvap	52.91	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.038		Crippen Method
mcvol	176.570	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1437.00		NIST Webbook
rinpol	1437.00		NIST Webbook
tb	603.16	K	Joback Method
tc	785.63	K	Joback Method
tf	375.63	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.68	J/mol×K	603.16	Joback Method
cpg	467.25	J/mol×K	633.57	Joback Method
cpg	479.14	J/mol×K	663.98	Joback Method
cpg	490.36	J/mol×K	694.39	Joback Method
cpg	500.94	J/mol×K	724.80	Joback Method
cpg	510.89	J/mol×K	755.22	Joback Method
cpg	520.21	J/mol×K	785.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357352&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