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

Inchi: InChI=1S/C10H7ClF4O2/c11-3-4-17-9(16)6-1-2-7(8(12)5-6)10(13,14)15/h1-2,5H,3-4H2
InchiKey: PPQCZTZJWICKQD-UHFFFAOYSA-N
Formula: C10H7ClF4O2
SMILES: O=C(OCCCl)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 270.61

Physical Properties

Property code	Value	Unit	Source
gf	-895.78	kJ/mol	Joback Method
hf	-1089.87	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	50.43	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.240		Crippen Method
mcvol	154.760	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	1408.00		NIST Webbook
rinpol	1408.00		NIST Webbook
tb	572.41	K	Joback Method
tc	764.45	K	Joback Method
tf	360.78	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.89	J/mol×K	572.41	Joback Method
cpg	372.46	J/mol×K	604.42	Joback Method
cpg	382.37	J/mol×K	636.42	Joback Method
cpg	391.65	J/mol×K	668.43	Joback Method
cpg	400.32	J/mol×K	700.43	Joback Method
cpg	408.39	J/mol×K	732.44	Joback Method
cpg	415.90	J/mol×K	764.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357350&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

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