4-Fluoro-3-trifluoromethylbenzoic acid, propyl ester

Inchi: InChI=1S/C11H10F4O2/c1-2-5-17-10(16)7-3-4-9(12)8(6-7)11(13,14)15/h3-4,6H,2,5H2,1H

InchiKey: SHZAOHRBTXAUTD-UHFFFAOYSA-N

Formula: C11H10F4O2

SMILES: CCCOC(=O)c1ccc(F)c(C(F)(F)F)c1

Mol. weight [g/mol]: 250.19

Physical Properties

Property code	Value	Unit	Source
gf	-875.43	kJ/mol	Joback Method
hf	-1094.77	kJ/mol	Joback Method
hfus	25.20	kJ/mol	Joback Method
hvap	48.27	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.411		Crippen Method
mcvol	156.610	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1242.00		NIST Webbook
rinpol	1242.00		NIST Webbook
tb	557.86	K	Joback Method
tc	743.16	K	Joback Method
tf	342.13	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.19	J/mol×K	557.86	Joback Method
cpg	394.31	J/mol×K	588.74	Joback Method
cpg	405.75	J/mol×K	619.63	Joback Method
cpg	416.53	J/mol×K	650.51	Joback Method
cpg	426.68	J/mol×K	681.40	Joback Method
cpg	436.21	J/mol×K	712.28	Joback Method
cpg	445.15	J/mol×K	743.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338914&Units=SI

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

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