5-Fluoro-2-trifluoromethylbenzoic acid, ethyl ester

Inchi: InChI=1S/C10H8F4O2/c1-2-16-9(15)7-5-6(11)3-4-8(7)10(12,13)14/h3-5H,2H2,1H3
InchiKey: XRUGEWMVTKVACF-UHFFFAOYSA-N
Formula: C10H8F4O2
SMILES: CCOC(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]: 236.16

Physical Properties

Property code	Value	Unit	Source
gf	-883.85	kJ/mol	Joback Method
hf	-1074.13	kJ/mol	Joback Method
hfus	22.61	kJ/mol	Joback Method
hvap	46.05	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.021		Crippen Method
mcvol	142.520	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
tb	534.98	K	Joback Method
tc	722.38	K	Joback Method
tf	330.86	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.59	J/mol×K	534.98	Joback Method
cpg	347.94	J/mol×K	566.21	Joback Method
cpg	358.64	J/mol×K	597.45	Joback Method
cpg	368.71	J/mol×K	628.68	Joback Method
cpg	378.18	J/mol×K	659.92	Joback Method
cpg	387.06	J/mol×K	691.15	Joback Method
cpg	395.38	J/mol×K	722.38	Joback Method

Sources

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=U338736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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