3-Fluoro-4-trifluoromethylbenzoic acid, methyl ester

Inchi: InChI=1S/C9H6F4O2/c1-15-8(14)5-2-3-6(7(10)4-5)9(11,12)13/h2-4H,1H3
InchiKey: NLARJSCTWHCNMQ-UHFFFAOYSA-N
Formula: C9H6F4O2
SMILES: COC(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 222.14

Physical Properties

Property code	Value	Unit	Source
gf	-892.27	kJ/mol	Joback Method
hf	-1053.49	kJ/mol	Joback Method
hfus	20.02	kJ/mol	Joback Method
hvap	43.82	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.631		Crippen Method
mcvol	128.430	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
rinpol	1101.00		NIST Webbook
tb	512.10	K	Joback Method
tc	701.72	K	Joback Method
tf	319.59	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.78	J/mol×K	512.10	Joback Method
cpg	303.25	J/mol×K	543.70	Joback Method
cpg	313.11	J/mol×K	575.31	Joback Method
cpg	322.38	J/mol×K	606.91	Joback Method
cpg	331.08	J/mol×K	638.51	Joback Method
cpg	339.24	J/mol×K	670.11	Joback Method
cpg	346.86	J/mol×K	701.72	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=U357949&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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