5-Fluoro-3-trifluoromethylbenzoic acid, butyl ester

Inchi: InChI=1S/C12H12F4O2/c1-2-3-4-18-11(17)8-5-9(12(14,15)16)7-10(13)6-8/h5-7H,2-4H2,
InchiKey: LODQHGFOBHETPI-UHFFFAOYSA-N
Formula: C12H12F4O2
SMILES: CCCCOC(=O)c1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 264.22

Physical Properties

Property code	Value	Unit	Source
gf	-867.01	kJ/mol	Joback Method
hf	-1115.41	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	50.50	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.801		Crippen Method
mcvol	170.700	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1259.00		NIST Webbook
rinpol	1259.00		NIST Webbook
tb	580.74	K	Joback Method
tc	764.11	K	Joback Method
tf	353.40	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.48	J/mol×K	580.74	Joback Method
cpg	442.29	J/mol×K	611.30	Joback Method
cpg	454.38	J/mol×K	641.86	Joback Method
cpg	465.79	J/mol×K	672.43	Joback Method
cpg	476.53	J/mol×K	702.99	Joback Method
cpg	486.63	J/mol×K	733.55	Joback Method
cpg	496.11	J/mol×K	764.11	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=U338895&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