2-Fluoro-5-trifluoromethylbenzoic acid, nonyl ester

Inchi: InChI=1S/C17H22F4O2/c1-2-3-4-5-6-7-8-11-23-16(22)14-12-13(17(19,20)21)9-10-15(14
InchiKey: HLPBFRSEHXKADZ-UHFFFAOYSA-N
Formula: C17H22F4O2
SMILES: CCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]: 334.35

Physical Properties

Property code	Value	Unit	Source
gf	-824.91	kJ/mol	Joback Method
hf	-1218.61	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	61.63	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.752		Crippen Method
mcvol	241.150	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
tb	695.14	K	Joback Method
tc	873.15	K	Joback Method
tf	409.75	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.03	J/mol×K	695.14	Joback Method
cpg	703.30	J/mol×K	724.81	Joback Method
cpg	717.74	J/mol×K	754.48	Joback Method
cpg	731.37	J/mol×K	784.15	Joback Method
cpg	744.21	J/mol×K	813.81	Joback Method
cpg	756.32	J/mol×K	843.48	Joback Method
cpg	767.70	J/mol×K	873.15	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=U338963&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