2-Fluoro-5-trifluoromethylbenzoic acid, decyl ester

Inchi: InChI=1S/C18H24F4O2/c1-2-3-4-5-6-7-8-9-12-24-17(23)15-13-14(18(20,21)22)10-11-16

InchiKey: QCKDMXZOUFMVNG-UHFFFAOYSA-N

Formula: C18H24F4O2

SMILES: CCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]: 348.38

Physical Properties

Property code	Value	Unit	Source
gf	-816.49	kJ/mol	Joback Method
hf	-1239.25	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	63.85	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.142		Crippen Method
mcvol	255.240	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	718.02	K	Joback Method
tc	896.17	K	Joback Method
tf	421.02	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.55	J/mol×K	718.02	Joback Method
cpg	759.20	J/mol×K	747.71	Joback Method
cpg	774.00	J/mol×K	777.40	Joback Method
cpg	787.96	J/mol×K	807.10	Joback Method
cpg	801.12	J/mol×K	836.79	Joback Method
cpg	813.51	J/mol×K	866.48	Joback Method
cpg	825.17	J/mol×K	896.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338964&Units=SI
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

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