4-Fluoro-2-trifluoromethylbenzoic acid, undecyl ester

Inchi: InChI=1S/C19H26F4O2/c1-2-3-4-5-6-7-8-9-10-13-25-18(24)16-12-11-15(20)14-17(16)19

InchiKey: DZFFBCFURBDZOL-UHFFFAOYSA-N

Formula: C19H26F4O2

SMILES: CCCCCCCCCCCOC(=O)c1ccc(F)cc1C(F)(F)F

Mol. weight [g/mol]: 362.40

Physical Properties

Property code	Value	Unit	Source
gf	-808.07	kJ/mol	Joback Method
hf	-1259.89	kJ/mol	Joback Method
hfus	45.92	kJ/mol	Joback Method
hvap	66.08	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.532		Crippen Method
mcvol	269.330	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinpol	2017.00		NIST Webbook
rinpol	2017.00		NIST Webbook
tb	740.90	K	Joback Method
tc	919.72	K	Joback Method
tf	432.29	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.14	J/mol×K	740.90	Joback Method
cpg	816.18	J/mol×K	770.70	Joback Method
cpg	831.31	J/mol×K	800.51	Joback Method
cpg	845.59	J/mol×K	830.31	Joback Method
cpg	859.04	J/mol×K	860.11	Joback Method
cpg	871.71	J/mol×K	889.92	Joback Method
cpg	883.62	J/mol×K	919.72	Joback Method

Sources

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=U338828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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