4-Fluoro-2-trifluoromethylbenzoic acid, tridecyl ester

Inchi: InChI=1S/C21H30F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-15-27-20(26)18-14-13-17(22)16-19

InchiKey: KNJJHWUGZXIWOR-UHFFFAOYSA-N

Formula: C21H30F4O2

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

Mol. weight [g/mol]: 390.46

Physical Properties

Property code	Value	Unit	Source
gf	-791.23	kJ/mol	Joback Method
hf	-1301.17	kJ/mol	Joback Method
hfus	51.10	kJ/mol	Joback Method
hvap	70.53	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.312		Crippen Method
mcvol	297.510	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	786.66	K	Joback Method
tc	968.61	K	Joback Method
tf	454.83	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.29	J/mol×K	786.66	Joback Method
cpg	933.08	J/mol×K	816.98	Joback Method
cpg	948.90	J/mol×K	847.31	Joback Method
cpg	963.80	J/mol×K	877.63	Joback Method
cpg	977.82	J/mol×K	907.96	Joback Method
cpg	991.00	J/mol×K	938.28	Joback Method
cpg	1003.38	J/mol×K	968.61	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=U338830&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