5-Fluoro-2-trifluoromethylbenzoic acid, 5-tridecyl ester

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

InchiKey: DDLJOAGENLFHAV-UHFFFAOYSA-N

Formula: C21H30F4O2

SMILES: CCCCCCCCC(CCCC)OC(=O)c1cc(F)ccc1C(F)(F)F

Mol. weight [g/mol]: 390.46

Physical Properties

Property code	Value	Unit	Source
gf	-793.67	kJ/mol	Joback Method
hf	-1306.45	kJ/mol	Joback Method
hfus	47.58	kJ/mol	Joback Method
hvap	70.14	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.311		Crippen Method
mcvol	297.510	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2054.00		NIST Webbook
rinpol	2054.00		NIST Webbook
tb	786.22	K	Joback Method
tc	969.32	K	Joback Method
tf	439.83	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.79	J/mol×K	786.22	Joback Method
cpg	933.69	J/mol×K	816.74	Joback Method
cpg	949.60	J/mol×K	847.25	Joback Method
cpg	964.57	J/mol×K	877.77	Joback Method
cpg	978.65	J/mol×K	908.29	Joback Method
cpg	991.86	J/mol×K	938.80	Joback Method
cpg	1004.26	J/mol×K	969.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338551&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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