4-Fluoro-2-trifluromethylbenzoic acid, 2-pentadecyl ester

Inchi: InChI=1S/C23H34F4O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-18(2)29-22(28)20-16-15-19(24

InchiKey: RPTUEGRGBAHNEW-UHFFFAOYSA-N

Formula: C23H34F4O2

SMILES: CCCCCCCCCCCCCC(C)OC(=O)c1ccc(F)cc1C(F)(F)F

Mol. weight [g/mol]: 418.51

Physical Properties

Property code	Value	Unit	Source
gf	-776.83	kJ/mol	Joback Method
hf	-1347.73	kJ/mol	Joback Method
hfus	52.76	kJ/mol	Joback Method
hvap	74.60	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.091		Crippen Method
mcvol	325.690	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpol	2346.00		NIST Webbook
rinpol	2346.00		NIST Webbook
tb	831.98	K	Joback Method
tc	1020.35	K	Joback Method
tf	462.37	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.41	J/mol×K	831.98	Joback Method
cpg	1054.07	J/mol×K	863.38	Joback Method
cpg	1070.65	J/mol×K	894.77	Joback Method
cpg	1086.22	J/mol×K	926.17	Joback Method
cpg	1100.83	J/mol×K	957.56	Joback Method
cpg	1114.52	J/mol×K	988.96	Joback Method
cpg	1127.34	J/mol×K	1020.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338504&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