4-Fluoro-3-trifluoromethylbenzoic acid, pentadecyl ester

Inchi: InChI=1S/C23H34F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-29-22(28)19-15-16-21(24

InchiKey: FPJLPWZWGANMBV-UHFFFAOYSA-N

Formula: C23H34F4O2

SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccc(F)c(C(F)(F)F)c1

Mol. weight [g/mol]: 418.51

Physical Properties

Property code	Value	Unit	Source
gf	-774.39	kJ/mol	Joback Method
hf	-1342.45	kJ/mol	Joback Method
hfus	56.28	kJ/mol	Joback Method
hvap	74.98	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	8.093		Crippen Method
mcvol	325.690	ml/mol	McGowan Method
pc	952.60	kPa	Joback Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook
tb	832.42	K	Joback Method
tc	1020.27	K	Joback Method
tf	477.37	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.93	J/mol×K	832.42	Joback Method
cpg	1053.54	J/mol×K	863.73	Joback Method
cpg	1070.10	J/mol×K	895.04	Joback Method
cpg	1085.65	J/mol×K	926.34	Joback Method
cpg	1100.26	J/mol×K	957.65	Joback Method
cpg	1113.96	J/mol×K	988.96	Joback Method
cpg	1126.81	J/mol×K	1020.27	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=U338927&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