4-Fluoro-3-trifluoromethylbenzoic acid, tetradecyl ester

Inchi: InChI=1S/C22H32F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-28-21(27)18-14-15-20(23)19

InchiKey: LIWIOMGMKXQQRM-UHFFFAOYSA-N

Formula: C22H32F4O2

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

Mol. weight [g/mol]: 404.48

Physical Properties

Property code	Value	Unit	Source
gf	-782.81	kJ/mol	Joback Method
hf	-1321.81	kJ/mol	Joback Method
hfus	53.69	kJ/mol	Joback Method
hvap	72.76	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.702		Crippen Method
mcvol	311.600	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2324.00		NIST Webbook
rinpol	2324.00		NIST Webbook
tb	809.54	K	Joback Method
tc	994.06	K	Joback Method
tf	466.10	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.71	J/mol×K	809.54	Joback Method
cpg	992.89	J/mol×K	840.29	Joback Method
cpg	1009.07	J/mol×K	871.05	Joback Method
cpg	1024.29	J/mol×K	901.80	Joback Method
cpg	1038.60	J/mol×K	932.55	Joback Method
cpg	1052.04	J/mol×K	963.31	Joback Method
cpg	1064.65	J/mol×K	994.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338926&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