3-Fluoro-5-trifluoromethylbenzoic acid, 3-tetradecyl ester

Inchi: InChI=1S/C22H32F4O2/c1-3-5-6-7-8-9-10-11-12-13-20(4-2)28-21(27)17-14-18(22(24,25
InchiKey: HZIJHRJTFNLCJM-UHFFFAOYSA-N
Formula: C22H32F4O2
SMILES: CCCCCCCCCCCC(CC)OC(=O)c1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 404.48

Physical Properties

Property code	Value	Unit	Source
gf	-785.25	kJ/mol	Joback Method
hf	-1327.09	kJ/mol	Joback Method
hfus	50.17	kJ/mol	Joback Method
hvap	72.37	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.701		Crippen Method
mcvol	311.600	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2114.00		NIST Webbook
rinpol	2114.00		NIST Webbook
tb	809.10	K	Joback Method
tc	994.47	K	Joback Method
tf	451.10	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.20	J/mol×K	809.10	Joback Method
cpg	993.46	J/mol×K	839.99	Joback Method
cpg	1009.71	J/mol×K	870.89	Joback Method
cpg	1024.97	J/mol×K	901.78	Joback Method
cpg	1039.30	J/mol×K	932.68	Joback Method
cpg	1052.75	J/mol×K	963.57	Joback Method
cpg	1065.36	J/mol×K	994.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338665&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