4-Fluoro-3-trifluoromethylbenzoic acid, 3-hexadecyl ester

Inchi: InChI=1S/C24H36F4O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-20(4-2)30-23(29)19-16-17-22

InchiKey: AJBSNESMQNYYKI-UHFFFAOYSA-N

Formula: C24H36F4O2

SMILES: CCCCCCCCCCCCCC(CC)OC(=O)c1ccc(F)c(C(F)(F)F)c1

Mol. weight [g/mol]: 432.54

Physical Properties

Property code	Value	Unit	Source
gf	-768.41	kJ/mol	Joback Method
hf	-1368.37	kJ/mol	Joback Method
hfus	55.35	kJ/mol	Joback Method
hvap	76.82	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.481		Crippen Method
mcvol	339.780	ml/mol	McGowan Method
pc	902.89	kPa	Joback Method
rinpol	2394.00		NIST Webbook
rinpol	2394.00		NIST Webbook
tb	854.86	K	Joback Method
tc	1047.04	K	Joback Method
tf	473.64	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1097.37	J/mol×K	854.86	Joback Method
cpg	1115.45	J/mol×K	886.89	Joback Method
cpg	1132.40	J/mol×K	918.92	Joback Method
cpg	1148.30	J/mol×K	950.95	Joback Method
cpg	1163.19	J/mol×K	982.98	Joback Method
cpg	1177.13	J/mol×K	1015.01	Joback Method
cpg	1190.17	J/mol×K	1047.04	Joback Method

Sources

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=U338695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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