4-Fluoro-2-trifluoromethylbenzoic acid, hexadecyl ester

Inchi: InChI=1S/C24H36F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-30-23(29)21-17-16-20

InchiKey: LDGKTXNLCRIWJA-UHFFFAOYSA-N

Formula: C24H36F4O2

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(F)cc1C(F)(F)F

Mol. weight [g/mol]: 432.54

Physical Properties

Property code	Value	Unit	Source
gf	-765.97	kJ/mol	Joback Method
hf	-1363.09	kJ/mol	Joback Method
hfus	58.87	kJ/mol	Joback Method
hvap	77.21	kJ/mol	Joback Method
log10ws	-9.43		Crippen Method
logp	8.483		Crippen Method
mcvol	339.780	ml/mol	McGowan Method
pc	898.56	kPa	Joback Method
rinpol	2514.00		NIST Webbook
rinpol	2514.00		NIST Webbook
tb	855.30	K	Joback Method
tc	1047.30	K	Joback Method
tf	488.64	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.90	J/mol×K	855.30	Joback Method
cpg	1114.97	J/mol×K	887.30	Joback Method
cpg	1131.93	J/mol×K	919.30	Joback Method
cpg	1147.85	J/mol×K	951.30	Joback Method
cpg	1162.76	J/mol×K	983.30	Joback Method
cpg	1176.74	J/mol×K	1015.30	Joback Method
cpg	1189.84	J/mol×K	1047.30	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=U338833&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