3-Fluoro-4-trifluoromethylbenzoic acid, 6-chlorohexyl ester

Inchi: InChI=1S/C14H15ClF4O2/c15-7-3-1-2-4-8-21-13(20)10-5-6-11(12(16)9-10)14(17,18)19/h
InchiKey: SOYROGXPZXSKRC-UHFFFAOYSA-N
Formula: C14H15ClF4O2
SMILES: O=C(OCCCCCCCl)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 326.71

Physical Properties

Property code	Value	Unit	Source
gf	-862.10	kJ/mol	Joback Method
hf	-1172.43	kJ/mol	Joback Method
hfus	37.17	kJ/mol	Joback Method
hvap	59.33	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.801		Crippen Method
mcvol	211.120	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	1843.00		NIST Webbook
tb	663.93	K	Joback Method
tc	848.47	K	Joback Method
tf	405.86	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.05	J/mol×K	663.93	Joback Method
cpg	570.09	J/mol×K	694.69	Joback Method
cpg	582.36	J/mol×K	725.44	Joback Method
cpg	593.89	J/mol×K	756.20	Joback Method
cpg	604.71	J/mol×K	786.95	Joback Method
cpg	614.84	J/mol×K	817.71	Joback Method
cpg	624.33	J/mol×K	848.47	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=U357354&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