6-Fluoro-2-trifluoromethylbenzoic acid, isohexyl ester

Inchi: InChI=1S/C14H16F4O2/c1-9(2)5-4-8-20-13(19)12-10(14(16,17)18)6-3-7-11(12)15/h3,6-7
InchiKey: QTKFXNWPRGSAML-UHFFFAOYSA-N
Formula: C14H16F4O2
SMILES: CC(C)CCCOC(=O)c1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 292.27

Physical Properties

Property code	Value	Unit	Source
gf	-852.61	kJ/mol	Joback Method
hf	-1161.97	kJ/mol	Joback Method
hfus	29.45	kJ/mol	Joback Method
hvap	54.56	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.438		Crippen Method
mcvol	198.880	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
tb	626.06	K	Joback Method
tc	809.25	K	Joback Method
tf	360.94	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.19	J/mol×K	626.06	Joback Method
cpg	543.41	J/mol×K	656.59	Joback Method
cpg	556.84	J/mol×K	687.12	Joback Method
cpg	569.49	J/mol×K	717.66	Joback Method
cpg	581.39	J/mol×K	748.19	Joback Method
cpg	592.58	J/mol×K	778.72	Joback Method
cpg	603.08	J/mol×K	809.25	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=U338979&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