5-Fluoro-2-trifluoromethylbenzoic acid, cyclohexyl ester

Inchi: InChI=1S/C14H14F4O2/c15-9-6-7-12(14(16,17)18)11(8-9)13(19)20-10-4-2-1-3-5-10/h6-8

InchiKey: QDDYPHJZJWAPLF-UHFFFAOYSA-N

Formula: C14H14F4O2

SMILES: O=C(OC1CCCCC1)c1cc(F)ccc1C(F)(F)F

Mol. weight [g/mol]: 290.25

Physical Properties

Property code	Value	Unit	Source
gf	-825.72	kJ/mol	Joback Method
hf	-1102.37	kJ/mol	Joback Method
hfus	24.81	kJ/mol	Joback Method
hvap	55.38	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.334		Crippen Method
mcvol	188.020	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1574.00		NIST Webbook
tb	646.05	K	Joback Method
tc	854.74	K	Joback Method
tf	383.32	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.97	J/mol×K	646.05	Joback Method
cpg	536.42	J/mol×K	680.83	Joback Method
cpg	551.73	J/mol×K	715.61	Joback Method
cpg	565.93	J/mol×K	750.39	Joback Method
cpg	579.07	J/mol×K	785.17	Joback Method
cpg	591.19	J/mol×K	819.96	Joback Method
cpg	602.34	J/mol×K	854.74	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357626&Units=SI

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