2-Fluoro-6-trifluoromethylbenzoic acid, cyclohexylmethyl ester

Inchi: InChI=1S/C15H16F4O2/c16-12-8-4-7-11(15(17,18)19)13(12)14(20)21-9-10-5-2-1-3-6-10

InchiKey: IZGGPVIPRZWMDF-UHFFFAOYSA-N

Formula: C15H16F4O2

SMILES: O=C(OCC1CCCCC1)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 304.28

Physical Properties

Property code	Value	Unit	Source
gf	-817.30	kJ/mol	Joback Method
hf	-1123.01	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	57.61	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.582		Crippen Method
mcvol	202.110	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
tb	668.93	K	Joback Method
tc	874.62	K	Joback Method
tf	394.59	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.78	J/mol×K	668.93	Joback Method
cpg	589.53	J/mol×K	703.21	Joback Method
cpg	605.12	J/mol×K	737.49	Joback Method
cpg	619.61	J/mol×K	771.78	Joback Method
cpg	633.02	J/mol×K	806.06	Joback Method
cpg	645.41	J/mol×K	840.34	Joback Method
cpg	656.82	J/mol×K	874.62	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=U357695&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