Succinic acid, 2-fluoro-6-(trifluoromethyl)benzyl propyl ester

Inchi: InChI=1S/C15H16F4O4/c1-2-8-22-13(20)6-7-14(21)23-9-10-11(15(17,18)19)4-3-5-12(10

InchiKey: OFSRBTSSMHJSIT-UHFFFAOYSA-N

Formula: C15H16F4O4

SMILES: CCCOC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 336.28

Physical Properties

Property code	Value	Unit	Source
gf	-1075.67	kJ/mol	Joback Method
hf	-1422.13	kJ/mol	Joback Method
hfus	38.35	kJ/mol	Joback Method
hvap	66.33	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.621		Crippen Method
mcvol	220.410	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	725.67	K	Joback Method
tc	912.13	K	Joback Method
tf	459.37	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.46	J/mol×K	725.67	Joback Method
cpg	639.29	J/mol×K	756.75	Joback Method
cpg	651.32	J/mol×K	787.82	Joback Method
cpg	662.55	J/mol×K	818.90	Joback Method
cpg	673.02	J/mol×K	849.98	Joback Method
cpg	682.74	J/mol×K	881.05	Joback Method
cpg	691.73	J/mol×K	912.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381631&Units=SI
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

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