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

Inchi: InChI=1S/C14H14F4O4/c1-2-21-12(19)6-7-13(20)22-8-9-10(14(16,17)18)4-3-5-11(9)15/h

InchiKey: VHJWEZQDBMZUMI-UHFFFAOYSA-N

Formula: C14H14F4O4

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

Mol. weight [g/mol]: 322.25

Physical Properties

Property code	Value	Unit	Source
gf	-1084.09	kJ/mol	Joback Method
hf	-1401.49	kJ/mol	Joback Method
hfus	35.76	kJ/mol	Joback Method
hvap	64.11	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.231		Crippen Method
mcvol	206.320	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	702.79	K	Joback Method
tc	889.93	K	Joback Method
tf	448.10	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.36	J/mol×K	702.79	Joback Method
cpg	585.75	J/mol×K	733.98	Joback Method
cpg	597.37	J/mol×K	765.17	Joback Method
cpg	608.23	J/mol×K	796.36	Joback Method
cpg	618.35	J/mol×K	827.55	Joback Method
cpg	627.75	J/mol×K	858.74	Joback Method
cpg	636.44	J/mol×K	889.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381630&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