Succinic acid, ethyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C13H12F4O4/c1-2-20-10(18)6-7-11(19)21-9-5-3-4-8(12(9)14)13(15,16)17/h3-5

InchiKey: JBDUFFDZHWXXID-UHFFFAOYSA-N

Formula: C13H12F4O4

SMILES: CCOC(=O)CCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 308.23

Physical Properties

Property code	Value	Unit	Source
gf	-1092.51	kJ/mol	Joback Method
hf	-1380.85	kJ/mol	Joback Method
hfus	33.17	kJ/mol	Joback Method
hvap	61.88	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.093		Crippen Method
mcvol	192.230	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	1626.00		NIST Webbook
rinpol	1626.00		NIST Webbook
tb	679.91	K	Joback Method
tc	868.19	K	Joback Method
tf	436.83	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.50	J/mol×K	679.91	Joback Method
cpg	533.39	J/mol×K	711.29	Joback Method
cpg	544.55	J/mol×K	742.67	Joback Method
cpg	554.98	J/mol×K	774.05	Joback Method
cpg	564.71	J/mol×K	805.43	Joback Method
cpg	573.74	J/mol×K	836.81	Joback Method
cpg	582.10	J/mol×K	868.19	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=U390797&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