Succinic acid, 3-methylbut-2-en-1-yl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C16H16F4O4/c1-10(2)8-9-23-13(21)6-7-14(22)24-12-5-3-4-11(15(12)17)16(18

InchiKey: NNBYDSOYRGNLII-UHFFFAOYSA-N

Formula: C16H16F4O4

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

Mol. weight [g/mol]: 348.29

Physical Properties

Property code	Value	Unit	Source
gf	-995.58	kJ/mol	Joback Method
hf	-1335.34	kJ/mol	Joback Method
hfus	39.83	kJ/mol	Joback Method
hvap	68.60	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.040		Crippen Method
mcvol	230.200	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	1916.00		NIST Webbook
rinpol	1916.00		NIST Webbook
tb	752.59	K	Joback Method
tc	945.66	K	Joback Method
tf	451.60	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.79	J/mol×K	752.59	Joback Method
cpg	668.57	J/mol×K	784.77	Joback Method
cpg	680.51	J/mol×K	816.95	Joback Method
cpg	691.65	J/mol×K	849.12	Joback Method
cpg	702.01	J/mol×K	881.30	Joback Method
cpg	711.63	J/mol×K	913.48	Joback Method
cpg	720.55	J/mol×K	945.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390781&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

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