Succinic acid, 2-fluoro-6-(trifluoromethyl)benzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H24F4O4/c1-4-6-16(12(2)3)27-18(25)10-9-17(24)26-11-13-14(19(21,22)23
InchiKey: IJUZGZGDPMZVMR-UHFFFAOYSA-N
Formula: C19H24F4O4
SMILES: CCCC(OC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]: 392.39

Physical Properties

Property code	Value	Unit	Source
gf	-1046.87	kJ/mol	Joback Method
hf	-1515.25	kJ/mol	Joback Method
hfus	41.66	kJ/mol	Joback Method
hvap	74.46	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.036		Crippen Method
mcvol	276.770	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	816.31	K	Joback Method
tc	1008.25	K	Joback Method
tf	474.45	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.59	J/mol×K	816.31	Joback Method
cpg	865.13	J/mol×K	848.30	Joback Method
cpg	878.65	J/mol×K	880.29	Joback Method
cpg	891.20	J/mol×K	912.28	Joback Method
cpg	902.79	J/mol×K	944.27	Joback Method
cpg	913.47	J/mol×K	976.26	Joback Method
cpg	923.26	J/mol×K	1008.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381635&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