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

Inchi: InChI=1S/C16H18F4O4/c1-10(2)8-23-14(21)6-7-15(22)24-9-11-12(16(18,19)20)4-3-5-13

InchiKey: GASOVJGTMDHJRX-UHFFFAOYSA-N

Formula: C16H18F4O4

SMILES: CC(C)COC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 350.31

Physical Properties

Property code	Value	Unit	Source
gf	-1069.69	kJ/mol	Joback Method
hf	-1448.05	kJ/mol	Joback Method
hfus	37.42	kJ/mol	Joback Method
hvap	68.17	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.867		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	1871.00		NIST Webbook
rinpol	1871.00		NIST Webbook
tb	748.11	K	Joback Method
tc	936.51	K	Joback Method
tf	455.64	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.25	J/mol×K	748.11	Joback Method
cpg	694.65	J/mol×K	779.51	Joback Method
cpg	707.19	J/mol×K	810.91	Joback Method
cpg	718.87	J/mol×K	842.31	Joback Method
cpg	729.73	J/mol×K	873.71	Joback Method
cpg	739.78	J/mol×K	905.11	Joback Method
cpg	749.05	J/mol×K	936.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381632&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