Succinic acid, 2-methylhex-3-yl 2,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C18H23F3O4/c1-4-5-16(11(2)3)25-18(23)7-6-17(22)24-10-12-8-14(20)15(21)9

InchiKey: KJTBFSNNHQZGNX-UHFFFAOYSA-N

Formula: C18H23F3O4

SMILES: CCCC(OC(=O)CCC(=O)OCc1cc(F)c(F)cc1F)C(C)C

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-872.95	kJ/mol	Joback Method
hf	-1301.22	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	75.01	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.295		Crippen Method
mcvol	260.910	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
tb	802.37	K	Joback Method
tc	993.63	K	Joback Method
tf	472.69	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.45	J/mol×K	802.37	Joback Method
cpg	797.91	J/mol×K	834.25	Joback Method
cpg	811.40	J/mol×K	866.12	Joback Method
cpg	823.92	J/mol×K	898.00	Joback Method
cpg	835.50	J/mol×K	929.88	Joback Method
cpg	846.13	J/mol×K	961.75	Joback Method
cpg	855.82	J/mol×K	993.63	Joback Method

Sources

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=U382221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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