Succinic acid, 2-methylhex-3-yl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C19H25F3O5/c1-4-5-16(13(2)3)26-18(24)11-10-17(23)25-12-14-6-8-15(9-7-14

InchiKey: IJKQCMGRQGZFKS-UHFFFAOYSA-N

Formula: C19H25F3O5

SMILES: CCCC(OC(=O)CCC(=O)OCc1ccc(OC(F)(F)F)cc1)C(C)C

Mol. weight [g/mol]: 390.39

Physical Properties

Property code	Value	Unit	Source
gf	-947.43	kJ/mol	Joback Method
hf	-1439.89	kJ/mol	Joback Method
hfus	40.16	kJ/mol	Joback Method
hvap	77.03	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.776		Crippen Method
mcvol	280.870	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
tb	834.48	K	Joback Method
tc	1030.78	K	Joback Method
tf	483.57	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.55	J/mol×K	834.48	Joback Method
cpg	887.15	J/mol×K	867.20	Joback Method
cpg	900.63	J/mol×K	899.91	Joback Method
cpg	913.04	J/mol×K	932.63	Joback Method
cpg	924.39	J/mol×K	965.34	Joback Method
cpg	934.71	J/mol×K	998.06	Joback Method
cpg	944.02	J/mol×K	1030.78	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=U381564&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