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

Inchi: InChI=1S/C19H25F3O4/c1-4-7-16(13(2)3)26-18(24)11-10-17(23)25-12-14-8-5-6-9-15(14

InchiKey: NHTVCPFMNVEFMG-UHFFFAOYSA-N

Formula: C19H25F3O4

SMILES: CCCC(OC(=O)CCC(=O)OCc1ccccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 374.39

Physical Properties

Property code	Value	Unit	Source
gf	-842.43	kJ/mol	Joback Method
hf	-1307.67	kJ/mol	Joback Method
hfus	38.97	kJ/mol	Joback Method
hvap	74.62	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.897		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	2075.00		NIST Webbook
rinpol	2075.00		NIST Webbook
tb	812.06	K	Joback Method
tc	1006.99	K	Joback Method
tf	461.34	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.87	J/mol×K	812.06	Joback Method
cpg	858.88	J/mol×K	844.55	Joback Method
cpg	872.83	J/mol×K	877.04	Joback Method
cpg	885.78	J/mol×K	909.53	Joback Method
cpg	897.74	J/mol×K	942.01	Joback Method
cpg	908.77	J/mol×K	974.50	Joback Method
cpg	918.89	J/mol×K	1006.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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