Succinic acid, di(4-trifluoromethoxybenzyl) ester

Inchi: InChI=1S/C20H16F6O6/c21-19(22,23)31-15-5-1-13(2-6-15)11-29-17(27)9-10-18(28)30-1

InchiKey: ORJUIAPHKVLTSL-UHFFFAOYSA-N

Formula: C20H16F6O6

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

Mol. weight [g/mol]: 466.33

Physical Properties

Property code	Value	Unit	Source
gf	-1517.94	kJ/mol	Joback Method
hf	-1954.21	kJ/mol	Joback Method
hfus	46.46	kJ/mol	Joback Method
hvap	81.63	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.051		Crippen Method
mcvol	282.380	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2284.00		NIST Webbook
rinpol	2284.00		NIST Webbook
tb	906.90	K	Joback Method
tc	1115.36	K	Joback Method
tf	590.20	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.16	J/mol×K	906.90	Joback Method
cpg	889.92	J/mol×K	941.64	Joback Method
cpg	899.52	J/mol×K	976.39	Joback Method
cpg	908.02	J/mol×K	1011.13	Joback Method
cpg	915.44	J/mol×K	1045.88	Joback Method
cpg	921.83	J/mol×K	1080.62	Joback Method
cpg	927.24	J/mol×K	1115.36	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=U381566&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