Succinic acid, di(4-trifluoromethylbenzyl) ester

Inchi: InChI=1S/C20H16F6O4/c21-19(22,23)15-5-1-13(2-6-15)11-29-17(27)9-10-18(28)30-12-1
InchiKey: DURRPWYBGVCZMH-UHFFFAOYSA-N
Formula: C20H16F6O4
SMILES: O=C(CCC(=O)OCc1ccc(C(F)(F)F)cc1)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 434.33

Physical Properties

Property code	Value	Unit	Source
gf	-1307.94	kJ/mol	Joback Method
hf	-1689.77	kJ/mol	Joback Method
hfus	44.09	kJ/mol	Joback Method
hvap	76.81	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.291		Crippen Method
mcvol	270.640	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook
tb	862.06	K	Joback Method
tc	1067.07	K	Joback Method
tf	545.74	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.70	J/mol×K	862.06	Joback Method
cpg	838.49	J/mol×K	896.23	Joback Method
cpg	849.27	J/mol×K	930.40	Joback Method
cpg	859.12	J/mol×K	964.56	Joback Method
cpg	868.10	J/mol×K	998.73	Joback Method
cpg	876.28	J/mol×K	1032.90	Joback Method
cpg	883.72	J/mol×K	1067.07	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=U382451&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