Succinic acid, di(2-fluoro-6-(trifluoromethyl)benzyl) ester

Inchi: InChI=1S/C20H14F8O4/c21-15-5-1-3-13(19(23,24)25)11(15)9-31-17(29)7-8-18(30)32-10

InchiKey: QVKACRHMYNCIPA-UHFFFAOYSA-N

Formula: C20H14F8O4

SMILES: O=C(CCC(=O)OCc1c(F)cccc1C(F)(F)F)OCc1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 470.31

Physical Properties

Property code	Value	Unit	Source
gf	-1716.82	kJ/mol	Joback Method
hf	-2104.93	kJ/mol	Joback Method
hfus	49.47	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.569		Crippen Method
mcvol	274.180	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	870.56	K	Joback Method
tc	1070.54	K	Joback Method
tf	571.96	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.75	J/mol×K	870.56	Joback Method
cpg	849.78	J/mol×K	903.89	Joback Method
cpg	859.86	J/mol×K	937.22	Joback Method
cpg	869.05	J/mol×K	970.55	Joback Method
cpg	877.41	J/mol×K	1003.88	Joback Method
cpg	884.97	J/mol×K	1037.21	Joback Method
cpg	891.80	J/mol×K	1070.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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