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

Inchi: InChI=1S/C29H44F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-36-27(34)20-21-28
InchiKey: QCPXAIZVCGYFLP-UHFFFAOYSA-N
Formula: C29H44F4O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 532.65

Physical Properties

Property code	Value	Unit	Source
gf	-957.79	kJ/mol	Joback Method
hf	-1711.09	kJ/mol	Joback Method
hfus	74.61	kJ/mol	Joback Method
hvap	97.50	kJ/mol	Joback Method
log10ws	-10.30		Crippen Method
logp	9.082		Crippen Method
mcvol	417.670	ml/mol	McGowan Method
pc	703.59	kPa	Joback Method
rinpol	3204.00		NIST Webbook
rinpol	3204.00		NIST Webbook
tb	1045.99	K	Joback Method
tc	1303.14	K	Joback Method
tf	617.15	K	Joback Method
vc	1.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1458.43	J/mol×K	1045.99	Joback Method
cpg	1477.51	J/mol×K	1088.85	Joback Method
cpg	1494.66	J/mol×K	1131.71	Joback Method
cpg	1510.01	J/mol×K	1174.56	Joback Method
cpg	1523.68	J/mol×K	1217.42	Joback Method
cpg	1535.81	J/mol×K	1260.28	Joback Method
cpg	1546.53	J/mol×K	1303.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381647&Units=SI

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

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