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

Inchi: InChI=1S/C28H42F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21-35-26(33)19-20-27(34
InchiKey: PXXNUWAXWWHFQQ-UHFFFAOYSA-N
Formula: C28H42F4O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 518.62

Physical Properties

Property code	Value	Unit	Source
gf	-966.21	kJ/mol	Joback Method
hf	-1690.45	kJ/mol	Joback Method
hfus	72.02	kJ/mol	Joback Method
hvap	95.27	kJ/mol	Joback Method
log10ws	-9.88		Crippen Method
logp	8.692		Crippen Method
mcvol	403.580	ml/mol	McGowan Method
pc	740.84	kPa	Joback Method
rinpol	3106.00		NIST Webbook
rinpol	3106.00		NIST Webbook
tb	1023.11	K	Joback Method
tc	1268.10	K	Joback Method
tf	605.88	K	Joback Method
vc	1.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.32	J/mol×K	1023.11	Joback Method
cpg	1413.75	J/mol×K	1063.94	Joback Method
cpg	1430.41	J/mol×K	1104.77	Joback Method
cpg	1445.41	J/mol×K	1145.60	Joback Method
cpg	1458.86	J/mol×K	1186.44	Joback Method
cpg	1470.86	J/mol×K	1227.27	Joback Method
cpg	1481.52	J/mol×K	1268.10	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=U381646&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