Succinic acid, 2,5-difluorobenzyl heptadecyl ester

Inchi: InChI=1S/C28H44F2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-33-27(31)19-20-28
InchiKey: WKDAIVBOCAAROX-UHFFFAOYSA-N
Formula: C28H44F2O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 482.64

Physical Properties

Property code	Value	Unit	Source
gf	-579.43	kJ/mol	Joback Method
hf	-1289.48	kJ/mol	Joback Method
hfus	73.27	kJ/mol	Joback Method
hvap	98.20	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	8.203		Crippen Method
mcvol	400.040	ml/mol	McGowan Method
pc	770.32	kPa	Joback Method
rinpol	3207.00		NIST Webbook
rinpol	3207.00		NIST Webbook
tb	1027.80	K	Joback Method
tc	1270.92	K	Joback Method
tf	602.28	K	Joback Method
vc	1.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1382.17	J/mol×K	1027.80	Joback Method
cpg	1400.49	J/mol×K	1068.32	Joback Method
cpg	1416.87	J/mol×K	1108.84	Joback Method
cpg	1431.40	J/mol×K	1149.36	Joback Method
cpg	1444.13	J/mol×K	1189.88	Joback Method
cpg	1455.14	J/mol×K	1230.40	Joback Method
cpg	1464.51	J/mol×K	1270.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381232&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

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