Sebacic acid, 3,5-difluorophenyl tridecyl ester

Inchi: InChI=1S/C29H46F2O4/c1-2-3-4-5-6-7-8-9-12-15-18-21-34-28(32)19-16-13-10-11-14-17
InchiKey: LYCMWKVYKGYDKP-UHFFFAOYSA-N
Formula: C29H46F2O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 496.67

Physical Properties

Property code	Value	Unit	Source
gf	-571.01	kJ/mol	Joback Method
hf	-1310.12	kJ/mol	Joback Method
hfus	75.86	kJ/mol	Joback Method
hvap	100.43	kJ/mol	Joback Method
log10ws	-10.10		Crippen Method
logp	8.845		Crippen Method
mcvol	414.130	ml/mol	McGowan Method
pc	730.86	kPa	Joback Method
rinpol	3368.00		NIST Webbook
rinpol	3368.00		NIST Webbook
tb	1050.68	K	Joback Method
tc	1305.28	K	Joback Method
tf	613.55	K	Joback Method
vc	1.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1445.41	J/mol×K	1050.68	Joback Method
cpg	1464.22	J/mol×K	1093.11	Joback Method
cpg	1480.90	J/mol×K	1135.55	Joback Method
cpg	1495.53	J/mol×K	1177.98	Joback Method
cpg	1508.22	J/mol×K	1220.41	Joback Method
cpg	1519.04	J/mol×K	1262.85	Joback Method
cpg	1528.09	J/mol×K	1305.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354535&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