Sebacic acid, 2,3,6-trifluorobenzyl undecyl ester

Inchi: InChI=1S/C28H43F3O4/c1-2-3-4-5-6-7-10-13-16-21-34-26(32)17-14-11-8-9-12-15-18-27

InchiKey: JIIFDPCHIRVWJG-UHFFFAOYSA-N

Formula: C28H43F3O4

SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)ccc(F)c1F

Mol. weight [g/mol]: 500.63

Physical Properties

Property code	Value	Unit	Source
gf	-783.87	kJ/mol	Joback Method
hf	-1497.06	kJ/mol	Joback Method
hfus	75.96	kJ/mol	Joback Method
hvap	98.04	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	8.342		Crippen Method
mcvol	401.810	ml/mol	McGowan Method
pc	745.29	kPa	Joback Method
rinpol	3214.00		NIST Webbook
rinpol	3214.00		NIST Webbook
tb	1032.05	K	Joback Method
tc	1281.55	K	Joback Method
tf	615.39	K	Joback Method
vc	1.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1388.07	J/mol×K	1032.05	Joback Method
cpg	1406.41	J/mol×K	1073.63	Joback Method
cpg	1422.69	J/mol×K	1115.22	Joback Method
cpg	1436.97	J/mol×K	1156.80	Joback Method
cpg	1449.32	J/mol×K	1198.38	Joback Method
cpg	1459.81	J/mol×K	1239.97	Joback Method
cpg	1468.51	J/mol×K	1281.55	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=U380799&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