Sebacic acid, decyl 3,5-difluorophenyl ester

Inchi: InChI=1S/C26H40F2O4/c1-2-3-4-5-6-9-12-15-18-31-25(29)16-13-10-7-8-11-14-17-26(30
InchiKey: YYULLBWJIGKGAM-UHFFFAOYSA-N
Formula: C26H40F2O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 454.59

Physical Properties

Property code	Value	Unit	Source
gf	-596.27	kJ/mol	Joback Method
hf	-1248.20	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	93.75	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	7.675		Crippen Method
mcvol	371.860	ml/mol	McGowan Method
pc	859.48	kPa	Joback Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook
tb	982.04	K	Joback Method
tc	1206.32	K	Joback Method
tf	579.74	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.69	J/mol×K	982.04	Joback Method
cpg	1274.12	J/mol×K	1019.42	Joback Method
cpg	1289.93	J/mol×K	1056.80	Joback Method
cpg	1304.17	J/mol×K	1094.18	Joback Method
cpg	1316.89	J/mol×K	1131.56	Joback Method
cpg	1328.14	J/mol×K	1168.94	Joback Method
cpg	1337.96	J/mol×K	1206.32	Joback Method

Sources

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=U354532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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