Sebacic acid, 3,5-difluorophenyl nonyl ester

Inchi: InChI=1S/C25H38F2O4/c1-2-3-4-5-8-11-14-17-30-24(28)15-12-9-6-7-10-13-16-25(29)31
InchiKey: GKFZPKOESCWYQI-UHFFFAOYSA-N
Formula: C25H38F2O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 440.56

Physical Properties

Property code	Value	Unit	Source
gf	-604.69	kJ/mol	Joback Method
hf	-1227.56	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	91.52	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.285		Crippen Method
mcvol	357.770	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	2949.00		NIST Webbook
rinpol	2949.00		NIST Webbook
tb	959.16	K	Joback Method
tc	1175.88	K	Joback Method
tf	568.47	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1194.53	J/mol×K	959.16	Joback Method
cpg	1211.56	J/mol×K	995.28	Joback Method
cpg	1227.10	J/mol×K	1031.40	Joback Method
cpg	1241.18	J/mol×K	1067.52	Joback Method
cpg	1253.86	J/mol×K	1103.64	Joback Method
cpg	1265.16	J/mol×K	1139.76	Joback Method
cpg	1275.14	J/mol×K	1175.88	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354531&Units=SI

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