Sebacic acid, 3,5-difluorophenyl heptyl ester

Inchi: InChI=1S/C23H34F2O4/c1-2-3-4-9-12-15-28-22(26)13-10-7-5-6-8-11-14-23(27)29-21-17
InchiKey: WCGMOODEQBOBQR-UHFFFAOYSA-N
Formula: C23H34F2O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 412.51

Physical Properties

Property code	Value	Unit	Source
gf	-621.53	kJ/mol	Joback Method
hf	-1186.28	kJ/mol	Joback Method
hfus	60.32	kJ/mol	Joback Method
hvap	87.07	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	6.505		Crippen Method
mcvol	329.590	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	2759.00		NIST Webbook
rinpol	2759.00		NIST Webbook
tb	913.40	K	Joback Method
tc	1118.29	K	Joback Method
tf	545.93	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1071.65	J/mol×K	913.40	Joback Method
cpg	1087.95	J/mol×K	947.55	Joback Method
cpg	1102.97	J/mol×K	981.70	Joback Method
cpg	1116.72	J/mol×K	1015.84	Joback Method
cpg	1129.25	J/mol×K	1049.99	Joback Method
cpg	1140.57	J/mol×K	1084.14	Joback Method
cpg	1150.73	J/mol×K	1118.29	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=U354529&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