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

Inchi: InChI=1S/C22H31F3O4/c1-2-3-10-15-28-20(26)11-8-6-4-5-7-9-12-21(27)29-16-17-18(23
InchiKey: ZRJBMJLRKOVDHY-UHFFFAOYSA-N
Formula: C22H31F3O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 416.47

Physical Properties

Property code	Value	Unit	Source
gf	-834.39	kJ/mol	Joback Method
hf	-1373.22	kJ/mol	Joback Method
hfus	60.42	kJ/mol	Joback Method
hvap	84.69	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.001		Crippen Method
mcvol	317.270	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	2630.00		NIST Webbook
rinpol	2630.00		NIST Webbook
tb	894.77	K	Joback Method
tc	1095.50	K	Joback Method
tf	547.77	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.57	J/mol×K	894.77	Joback Method
cpg	1033.28	J/mol×K	928.23	Joback Method
cpg	1047.78	J/mol×K	961.68	Joback Method
cpg	1061.10	J/mol×K	995.14	Joback Method
cpg	1073.24	J/mol×K	1028.59	Joback Method
cpg	1084.23	J/mol×K	1062.05	Joback Method
cpg	1094.09	J/mol×K	1095.50	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=U380794&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