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

Inchi: InChI=1S/C23H33F3O4/c1-2-3-4-11-16-29-21(27)12-9-7-5-6-8-10-13-22(28)30-17-18-19
InchiKey: RHVNRJQNVFAIMN-UHFFFAOYSA-N
Formula: C23H33F3O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 430.50

Physical Properties

Property code	Value	Unit	Source
gf	-825.97	kJ/mol	Joback Method
hf	-1393.86	kJ/mol	Joback Method
hfus	63.01	kJ/mol	Joback Method
hvap	86.92	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	6.391		Crippen Method
mcvol	331.360	ml/mol	McGowan Method
pc	987.02	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	917.65	K	Joback Method
tc	1123.68	K	Joback Method
tf	559.04	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.10	J/mol×K	917.65	Joback Method
cpg	1094.20	J/mol×K	951.99	Joback Method
cpg	1108.99	J/mol×K	986.33	Joback Method
cpg	1122.50	J/mol×K	1020.67	Joback Method
cpg	1134.75	J/mol×K	1055.01	Joback Method
cpg	1145.77	J/mol×K	1089.34	Joback Method
cpg	1155.57	J/mol×K	1123.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380795&Units=SI
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

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