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

Inchi: InChI=1S/C20H27F3O4/c1-2-13-26-18(24)9-7-5-3-4-6-8-10-19(25)27-14-15-16(21)11-12
InchiKey: HIRWKAAUVLSIOO-UHFFFAOYSA-N
Formula: C20H27F3O4
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 388.42

Physical Properties

Property code	Value	Unit	Source
gf	-851.23	kJ/mol	Joback Method
hf	-1331.94	kJ/mol	Joback Method
hfus	55.24	kJ/mol	Joback Method
hvap	80.24	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.221		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2434.00		NIST Webbook
rinpol	2434.00		NIST Webbook
tb	849.01	K	Joback Method
tc	1041.90	K	Joback Method
tf	525.23	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.45	J/mol×K	849.01	Joback Method
cpg	913.42	J/mol×K	881.16	Joback Method
cpg	927.34	J/mol×K	913.31	Joback Method
cpg	940.22	J/mol×K	945.45	Joback Method
cpg	952.08	J/mol×K	977.60	Joback Method
cpg	962.94	J/mol×K	1009.75	Joback Method
cpg	972.79	J/mol×K	1041.90	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=U380791&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