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

Inchi: InChI=1S/C21H29F3O4/c1-15(2)13-27-19(25)9-7-5-3-4-6-8-10-20(26)28-14-16-17(22)11
InchiKey: MWHPKSLEFBJEIV-UHFFFAOYSA-N
Formula: C21H29F3O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 402.45

Physical Properties

Property code	Value	Unit	Source
gf	-845.25	kJ/mol	Joback Method
hf	-1357.86	kJ/mol	Joback Method
hfus	54.31	kJ/mol	Joback Method
hvap	82.07	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.467		Crippen Method
mcvol	303.180	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	871.45	K	Joback Method
tc	1068.27	K	Joback Method
tf	521.50	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.17	J/mol×K	871.45	Joback Method
cpg	973.52	J/mol×K	904.25	Joback Method
cpg	987.74	J/mol×K	937.06	Joback Method
cpg	1000.83	J/mol×K	969.86	Joback Method
cpg	1012.81	J/mol×K	1002.66	Joback Method
cpg	1023.71	J/mol×K	1035.47	Joback Method
cpg	1033.53	J/mol×K	1068.27	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=U380792&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