Sebacic acid, isobutyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C22H31F3O5/c1-17(2)15-28-20(26)9-7-5-3-4-6-8-10-21(27)29-16-18-11-13-19

InchiKey: LVVHCJCSPGHUQW-UHFFFAOYSA-N

Formula: C22H31F3O5

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 432.47

Physical Properties

Property code	Value	Unit	Source
gf	-919.73	kJ/mol	Joback Method
hf	-1496.53	kJ/mol	Joback Method
hfus	51.45	kJ/mol	Joback Method
hvap	84.09	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	5.948		Crippen Method
mcvol	323.140	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
rinpol	2389.00		NIST Webbook
rinpol	2389.00		NIST Webbook
tb	903.56	K	Joback Method
tc	1106.81	K	Joback Method
tf	532.38	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.27	J/mol×K	903.56	Joback Method
cpg	1064.56	J/mol×K	937.44	Joback Method
cpg	1078.59	J/mol×K	971.31	Joback Method
cpg	1091.40	J/mol×K	1005.19	Joback Method
cpg	1103.02	J/mol×K	1039.06	Joback Method
cpg	1113.49	J/mol×K	1072.94	Joback Method
cpg	1122.85	J/mol×K	1106.81	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=U416790&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