Sebacic acid, di(2,3,6-trifluorobenzyl) ester

Inchi: InChI=1S/C24H24F6O4/c25-17-9-11-19(27)23(29)15(17)13-33-21(31)7-5-3-1-2-4-6-8-22
InchiKey: OLTAGCTTXIXYCZ-UHFFFAOYSA-N
Formula: C24H24F6O4
SMILES: O=C(CCCCCCCCC(=O)OCc1c(F)ccc(F)c1F)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 490.44

Physical Properties

Property code	Value	Unit	Source
gf	-1318.46	kJ/mol	Joback Method
hf	-1800.71	kJ/mol	Joback Method
hfus	67.72	kJ/mol	Joback Method
hvap	90.95	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	6.429		Crippen Method
mcvol	327.000	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	2899.00		NIST Webbook
tb	979.96	K	Joback Method
tc	1201.06	K	Joback Method
tf	636.06	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1052.63	J/mol×K	979.96	Joback Method
cpg	1065.27	J/mol×K	1016.81	Joback Method
cpg	1076.46	J/mol×K	1053.66	Joback Method
cpg	1086.24	J/mol×K	1090.51	Joback Method
cpg	1094.63	J/mol×K	1127.36	Joback Method
cpg	1101.65	J/mol×K	1164.21	Joback Method
cpg	1107.32	J/mol×K	1201.06	Joback Method

Sources

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=U380800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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