Sebacic acid, butyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C22H31F3O5/c1-2-3-16-28-20(26)10-8-6-4-5-7-9-11-21(27)29-17-18-12-14-19

InchiKey: RVGQDRAEZIYRHD-UHFFFAOYSA-N

Formula: C22H31F3O5

SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 432.47

Physical Properties

Property code	Value	Unit	Source
gf	-917.29	kJ/mol	Joback Method
hf	-1491.25	kJ/mol	Joback Method
hfus	54.98	kJ/mol	Joback Method
hvap	84.48	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.092		Crippen Method
mcvol	323.140	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	2426.00		NIST Webbook
rinpol	2426.00		NIST Webbook
tb	904.00	K	Joback Method
tc	1107.01	K	Joback Method
tf	547.38	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.79	J/mol×K	904.00	Joback Method
cpg	1064.09	J/mol×K	937.83	Joback Method
cpg	1078.15	J/mol×K	971.67	Joback Method
cpg	1090.99	J/mol×K	1005.50	Joback Method
cpg	1102.66	J/mol×K	1039.34	Joback Method
cpg	1113.19	J/mol×K	1073.17	Joback Method
cpg	1122.63	J/mol×K	1107.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416791&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