Sebacic acid, di(4-trifluoromethoxybenzyl) ester

Inchi: InChI=1S/C26H28F6O6/c27-25(28,29)37-21-13-9-19(10-14-21)17-35-23(33)7-5-3-1-2-4-

InchiKey: JMHRXKACIBAHAX-UHFFFAOYSA-N

Formula: C26H28F6O6

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

Mol. weight [g/mol]: 550.49

Physical Properties

Property code	Value	Unit	Source
gf	-1467.42	kJ/mol	Joback Method
hf	-2078.05	kJ/mol	Joback Method
hfus	62.00	kJ/mol	Joback Method
hvap	94.98	kJ/mol	Joback Method
log10ws	-9.35		Crippen Method
logp	7.391		Crippen Method
mcvol	366.920	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	2759.00		NIST Webbook
rinpol	2759.00		NIST Webbook
tb	1044.18	K	Joback Method
tc	1282.70	K	Joback Method
tf	657.82	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.24	J/mol×K	1044.18	Joback Method
cpg	1242.22	J/mol×K	1083.93	Joback Method
cpg	1252.61	J/mol×K	1123.69	Joback Method
cpg	1261.51	J/mol×K	1163.44	Joback Method
cpg	1269.01	J/mol×K	1203.19	Joback Method
cpg	1275.20	J/mol×K	1242.94	Joback Method
cpg	1280.17	J/mol×K	1282.70	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=U416799&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