Glutaric acid, 1-phenyl-2,2,2-trifluoroethyl tetradecyl ester

Inchi: InChI=1S/C27H41F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-22-33-24(31)20-17-21-25(32)34

InchiKey: TWZKWJCVVBVJBX-UHFFFAOYSA-N

Formula: C27H41F3O4

SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 486.61

Physical Properties

Property code	Value	Unit	Source
gf	-763.00	kJ/mol	Joback Method
hf	-1456.04	kJ/mol	Joback Method
hfus	63.60	kJ/mol	Joback Method
hvap	92.15	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	8.248		Crippen Method
mcvol	387.720	ml/mol	McGowan Method
pc	818.66	kPa	Joback Method
tb	990.56	K	Joback Method
tc	1217.28	K	Joback Method
tf	553.98	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1327.43	J/mol×K	990.56	Joback Method
cpg	1345.21	J/mol×K	1028.35	Joback Method
cpg	1361.49	J/mol×K	1066.13	Joback Method
cpg	1376.36	J/mol×K	1103.92	Joback Method
cpg	1389.92	J/mol×K	1141.71	Joback Method
cpg	1402.26	J/mol×K	1179.49	Joback Method
cpg	1413.47	J/mol×K	1217.28	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=U377376&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume