Glutaric acid, 1-(pentafluorophenyl)ethyl tetradecyl ester

Inchi: InChI=1S/C27H39F5O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-35-20(33)16-15-17-21(34)3

InchiKey: NJYZWLSJRPZAOO-UHFFFAOYSA-N

Formula: C27H39F5O4

SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 522.59

Physical Properties

Property code	Value	Unit	Source
gf	-1203.61	kJ/mol	Joback Method
hf	-1896.86	kJ/mol	Joback Method
hfus	75.23	kJ/mol	Joback Method
hvap	95.12	kJ/mol	Joback Method
log10ws	-10.07		Crippen Method
logp	8.401		Crippen Method
mcvol	391.260	ml/mol	McGowan Method
pc	738.82	kPa	Joback Method
rinpol	2911.00		NIST Webbook
rinpol	2911.00		NIST Webbook
tb	1017.23	K	Joback Method
tc	1266.02	K	Joback Method
tf	615.34	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1337.47	J/mol×K	1017.23	Joback Method
cpg	1355.15	J/mol×K	1058.69	Joback Method
cpg	1370.72	J/mol×K	1100.16	Joback Method
cpg	1384.23	J/mol×K	1141.62	Joback Method
cpg	1395.71	J/mol×K	1183.09	Joback Method
cpg	1405.23	J/mol×K	1224.55	Joback Method
cpg	1412.82	J/mol×K	1266.02	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=U377008&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