Glutaric acid, pentadecyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C27H40F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-34-23(32)16-15-17-24(33

InchiKey: MJTNIAMBFDNMGH-UHFFFAOYSA-N

Formula: C27H40F4O4

SMILES: CCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 504.60

Physical Properties

Property code	Value	Unit	Source
gf	-996.73	kJ/mol	Joback Method
hf	-1684.00	kJ/mol	Joback Method
hfus	76.06	kJ/mol	Joback Method
hvap	95.66	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.091		Crippen Method
mcvol	389.490	ml/mol	McGowan Method
pc	760.16	kPa	Joback Method
rinpol	3157.00		NIST Webbook
rinpol	3157.00		NIST Webbook
tb	1013.42	K	Joback Method
tc	1257.85	K	Joback Method
tf	617.23	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1331.25	J/mol×K	1013.42	Joback Method
cpg	1349.13	J/mol×K	1054.16	Joback Method
cpg	1365.02	J/mol×K	1094.90	Joback Method
cpg	1378.96	J/mol×K	1135.64	Joback Method
cpg	1391.01	J/mol×K	1176.37	Joback Method
cpg	1401.23	J/mol×K	1217.11	Joback Method
cpg	1409.67	J/mol×K	1257.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377453&Units=SI

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

Latest version available from:
https://www.chemeo.com/cid/115-854-6/Glutaric-acid-pentadecyl-2-3-4-5-tetrafluorobenzyl-ester.pdf
Generated by Cheméo on 2024-05-04 15:03:31.787631542 +0000 UTC m=+17124260.708208853.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.