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

Inchi: InChI=1S/C29H44F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-36-25(34)18-17-19

InchiKey: UQECECJPJFWUSV-UHFFFAOYSA-N

Formula: C29H44F4O4

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

Mol. weight [g/mol]: 532.65

Physical Properties

Property code	Value	Unit	Source
gf	-979.89	kJ/mol	Joback Method
hf	-1725.28	kJ/mol	Joback Method
hfus	81.25	kJ/mol	Joback Method
hvap	100.12	kJ/mol	Joback Method
log10ws	-10.61		Crippen Method
logp	8.871		Crippen Method
mcvol	417.670	ml/mol	McGowan Method
pc	685.65	kPa	Joback Method
rinpol	3359.00		NIST Webbook
rinpol	3359.00		NIST Webbook
tb	1059.18	K	Joback Method
tc	1330.17	K	Joback Method
tf	639.77	K	Joback Method
vc	1.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1456.84	J/mol×K	1059.18	Joback Method
cpg	1475.79	J/mol×K	1104.35	Joback Method
cpg	1492.25	J/mol×K	1149.51	Joback Method
cpg	1506.30	J/mol×K	1194.68	Joback Method
cpg	1518.02	J/mol×K	1239.84	Joback Method
cpg	1527.51	J/mol×K	1285.01	Joback Method
cpg	1534.85	J/mol×K	1330.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377455&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