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

Inchi: InChI=1S/C28H42F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-35-24(33)17-16-18-25

InchiKey: OBYJGIOTLDEOTQ-UHFFFAOYSA-N

Formula: C28H42F4O4

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

Mol. weight [g/mol]: 518.62

Physical Properties

Property code	Value	Unit	Source
gf	-988.31	kJ/mol	Joback Method
hf	-1704.64	kJ/mol	Joback Method
hfus	78.66	kJ/mol	Joback Method
hvap	97.89	kJ/mol	Joback Method
log10ws	-10.19		Crippen Method
logp	8.481		Crippen Method
mcvol	403.580	ml/mol	McGowan Method
pc	721.46	kPa	Joback Method
rinpol	3258.00		NIST Webbook
rinpol	3258.00		NIST Webbook
tb	1036.30	K	Joback Method
tc	1293.22	K	Joback Method
tf	628.50	K	Joback Method
vc	1.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1393.90	J/mol×K	1036.30	Joback Method
cpg	1412.31	J/mol×K	1079.12	Joback Method
cpg	1428.49	J/mol×K	1121.94	Joback Method
cpg	1442.51	J/mol×K	1164.76	Joback Method
cpg	1454.44	J/mol×K	1207.58	Joback Method
cpg	1464.35	J/mol×K	1250.40	Joback Method
cpg	1472.30	J/mol×K	1293.22	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=U377454&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