Glutaric acid, pentadecyl pentafluorobenzyl ester

Inchi: InChI=1S/C27H39F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-35-21(33)16-15-17-22(34

InchiKey: MOYCVPSQUDOPOT-UHFFFAOYSA-N

Formula: C27H39F5O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 522.59

Physical Properties

Property code	Value	Unit	Source
gf	-1201.17	kJ/mol	Joback Method
hf	-1891.58	kJ/mol	Joback Method
hfus	78.76	kJ/mol	Joback Method
hvap	95.51	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	8.230		Crippen Method
mcvol	391.260	ml/mol	McGowan Method
pc	735.62	kPa	Joback Method
rinpol	3068.00		NIST Webbook
rinpol	3068.00		NIST Webbook
tb	1017.67	K	Joback Method
tc	1269.31	K	Joback Method
tf	630.34	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1337.16	J/mol×K	1017.67	Joback Method
cpg	1355.11	J/mol×K	1059.61	Joback Method
cpg	1370.92	J/mol×K	1101.55	Joback Method
cpg	1384.63	J/mol×K	1143.49	Joback Method
cpg	1396.30	J/mol×K	1185.43	Joback Method
cpg	1405.97	J/mol×K	1227.37	Joback Method
cpg	1413.69	J/mol×K	1269.31	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=U358880&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