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

Inchi: InChI=1S/C22H30F4O4/c1-2-3-4-5-6-7-8-9-13-29-18(27)11-10-12-19(28)30-15-16-14-17

InchiKey: BYBZSDXPCGKVIC-UHFFFAOYSA-N

Formula: C22H30F4O4

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

Mol. weight [g/mol]: 434.46

Physical Properties

Property code	Value	Unit	Source
gf	-1038.83	kJ/mol	Joback Method
hf	-1580.80	kJ/mol	Joback Method
hfus	63.11	kJ/mol	Joback Method
hvap	84.53	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.140		Crippen Method
mcvol	319.040	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
rinpol	2645.00		NIST Webbook
rinpol	2645.00		NIST Webbook
tb	899.02	K	Joback Method
tc	1100.82	K	Joback Method
tf	560.88	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.05	J/mol×K	899.02	Joback Method
cpg	1039.56	J/mol×K	932.65	Joback Method
cpg	1053.85	J/mol×K	966.29	Joback Method
cpg	1066.93	J/mol×K	999.92	Joback Method
cpg	1078.81	J/mol×K	1033.55	Joback Method
cpg	1089.52	J/mol×K	1067.18	Joback Method
cpg	1099.06	J/mol×K	1100.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377448&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

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