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

Inchi: InChI=1S/C24H34F4O4/c1-2-3-4-5-6-7-8-9-10-11-15-31-20(29)13-12-14-21(30)32-17-18

InchiKey: OBQKIVJKUMYSEO-UHFFFAOYSA-N

Formula: C24H34F4O4

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

Mol. weight [g/mol]: 462.52

Physical Properties

Property code	Value	Unit	Source
gf	-1021.99	kJ/mol	Joback Method
hf	-1622.08	kJ/mol	Joback Method
hfus	68.30	kJ/mol	Joback Method
hvap	88.99	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	6.921		Crippen Method
mcvol	347.220	ml/mol	McGowan Method
pc	896.95	kPa	Joback Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		NIST Webbook
tb	944.78	K	Joback Method
tc	1160.06	K	Joback Method
tf	583.42	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.50	J/mol×K	944.78	Joback Method
cpg	1161.91	J/mol×K	980.66	Joback Method
cpg	1176.85	J/mol×K	1016.54	Joback Method
cpg	1190.34	J/mol×K	1052.42	Joback Method
cpg	1202.42	J/mol×K	1088.30	Joback Method
cpg	1213.10	J/mol×K	1124.18	Joback Method
cpg	1222.41	J/mol×K	1160.06	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=U377450&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