Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl isopropyl ester

Inchi: InChI=1S/C13H16F8O4/c1-7(2)25-9(23)5-3-4-8(22)24-6-11(16,17)13(20,21)12(18,19)10(

InchiKey: GOBWIYMYAUGXDE-UHFFFAOYSA-N

Formula: C13H16F8O4

SMILES: CC(C)OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 388.25

Physical Properties

Property code	Value	Unit	Source
gf	-1964.10	kJ/mol	Joback Method
hf	-2406.94	kJ/mol	Joback Method
hfus	30.35	kJ/mol	Joback Method
hvap	51.64	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.822		Crippen Method
mcvol	223.070	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	633.01	K	Joback Method
tc	790.69	K	Joback Method
tf	362.57	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.87	J/mol×K	633.01	Joback Method
cpg	654.83	J/mol×K	659.29	Joback Method
cpg	667.06	J/mol×K	685.57	Joback Method
cpg	678.58	J/mol×K	711.85	Joback Method
cpg	689.42	J/mol×K	738.13	Joback Method
cpg	699.62	J/mol×K	764.41	Joback Method
cpg	709.20	J/mol×K	790.69	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=U393367&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