Glutaric acid, tridec-2-yn-1-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C22H32F6O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-31-18(29)14-13-15-19(30)32-17

InchiKey: JYUQFHNDRBLZJX-UHFFFAOYSA-N

Formula: C22H32F6O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCC(F)(F)C(F)C(F)(F)F

Mol. weight [g/mol]: 474.48

Physical Properties

Property code	Value	Unit	Source
gf	-1296.30	kJ/mol	Joback Method
hf	-1914.15	kJ/mol	Joback Method
hfus	61.56	kJ/mol	Joback Method
hvap	77.15	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	6.313		Crippen Method
mcvol	337.740	ml/mol	McGowan Method
pc	917.16	kPa	Joback Method
rinpol	2345.00		NIST Webbook
tb	853.06	K	Joback Method
tc	1044.43	K	Joback Method
tf	581.50	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1086.22	J/mol×K	853.06	Joback Method
cpg	1102.81	J/mol×K	884.96	Joback Method
cpg	1118.33	J/mol×K	916.85	Joback Method
cpg	1132.83	J/mol×K	948.75	Joback Method
cpg	1146.37	J/mol×K	980.64	Joback Method
cpg	1159.00	J/mol×K	1012.54	Joback Method
cpg	1170.78	J/mol×K	1044.43	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=U393698&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