Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C22H30F8O4/c1-2-3-4-5-6-7-8-9-10-11-15-33-17(31)13-12-14-18(32)34-16-20

InchiKey: XFBXOELCRLNSRF-UHFFFAOYSA-N

Formula: C22H30F8O4

SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 510.46

Physical Properties

Property code	Value	Unit	Source
gf	-1683.08	kJ/mol	Joback Method
hf	-2315.12	kJ/mol	Joback Method
hfus	60.31	kJ/mol	Joback Method
hvap	74.22	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	6.558		Crippen Method
mcvol	341.280	ml/mol	McGowan Method
pc	878.96	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	848.37	K	Joback Method
tc	1038.98	K	Joback Method
tf	585.10	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.63	J/mol×K	848.37	Joback Method
cpg	1117.74	J/mol×K	880.14	Joback Method
cpg	1132.82	J/mol×K	911.91	Joback Method
cpg	1146.92	J/mol×K	943.67	Joback Method
cpg	1160.12	J/mol×K	975.44	Joback Method
cpg	1172.49	J/mol×K	1007.21	Joback Method
cpg	1184.10	J/mol×K	1038.98	Joback Method

Sources

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=U393939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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