Glutaric acid, di(dodec-9-ynyl) ester

Inchi: InChI=1S/C29H48O4/c1-3-5-7-9-11-13-15-17-19-21-26-32-28(30)24-23-25-29(31)33-27-
InchiKey: CUEYBQBFZWMGDC-UHFFFAOYSA-N
Formula: C29H48O4
SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCCCCCCCCC#CCC
Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	131.06	kJ/mol	Joback Method
hf	-586.89	kJ/mol	Joback Method
hfus	82.68	kJ/mol	Joback Method
hvap	102.76	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	7.531		Crippen Method
mcvol	417.150	ml/mol	McGowan Method
pc	775.91	kPa	Joback Method
rinpol	3471.00		NIST Webbook
tb	1033.50	K	Joback Method
tc	1270.93	K	Joback Method
tf	773.11	K	Joback Method
vc	1.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1425.97	J/mol×K	1033.50	Joback Method
cpg	1445.15	J/mol×K	1073.07	Joback Method
cpg	1462.52	J/mol×K	1112.64	Joback Method
cpg	1478.12	J/mol×K	1152.22	Joback Method
cpg	1492.02	J/mol×K	1191.79	Joback Method
cpg	1504.29	J/mol×K	1231.36	Joback Method
cpg	1514.97	J/mol×K	1270.93	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=U359796&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