Glutaric acid, dodec-2-en-1-yl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C29H50O4/c1-3-5-7-9-11-13-15-17-19-21-26-32-28(30)24-23-25-29(31)33-27-

InchiKey: PKHJGQNDYYCXQW-XUTLUUPISA-N

Formula: C29H50O4

SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCC=CCCCCCCCC

Mol. weight [g/mol]: 462.70

Physical Properties

Property code	Value	Unit	Source
gf	8.48	kJ/mol	Joback Method
hf	-741.97	kJ/mol	Joback Method
hfus	79.76	kJ/mol	Joback Method
hvap	100.57	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.084		Crippen Method
mcvol	421.450	ml/mol	McGowan Method
pc	731.25	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1028.66	K	Joback Method
tc	1269.82	K	Joback Method
tf	661.93	K	Joback Method
vc	1.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1454.73	J/mol×K	1028.66	Joback Method
cpg	1475.49	J/mol×K	1068.85	Joback Method
cpg	1494.52	J/mol×K	1109.05	Joback Method
cpg	1511.89	J/mol×K	1149.24	Joback Method
cpg	1527.69	J/mol×K	1189.43	Joback Method
cpg	1542.02	J/mol×K	1229.63	Joback Method
cpg	1554.97	J/mol×K	1269.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393947&Units=SI
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

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