Glutaric acid, non-5-yn-3-yl pentadecyl ester

Inchi: InChI=1S/C29H52O4/c1-4-7-9-11-12-13-14-15-16-17-18-19-21-26-32-28(30)24-22-25-29
InchiKey: QSFGRWNTBAWJGR-UHFFFAOYSA-N
Formula: C29H52O4
SMILES: CCCC#CCC(CC)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 464.72

Physical Properties

Property code	Value	Unit	Source
gf	-74.18	kJ/mol	Joback Method
hf	-864.47	kJ/mol	Joback Method
hfus	76.04	kJ/mol	Joback Method
hvap	100.22	kJ/mol	Joback Method
log10ws	-9.59		Crippen Method
logp	8.306		Crippen Method
mcvol	425.750	ml/mol	McGowan Method
pc	714.15	kPa	Joback Method
rinpol	3232.00		NIST Webbook
rinpol	3232.00		NIST Webbook
tb	1024.06	K	Joback Method
tc	1265.38	K	Joback Method
tf	652.01	K	Joback Method
vc	1.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1483.40	J/mol×K	1024.06	Joback Method
cpg	1504.29	J/mol×K	1064.28	Joback Method
cpg	1523.18	J/mol×K	1104.50	Joback Method
cpg	1540.16	J/mol×K	1144.72	Joback Method
cpg	1555.29	J/mol×K	1184.94	Joback Method
cpg	1568.64	J/mol×K	1225.16	Joback Method
cpg	1580.29	J/mol×K	1265.38	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=U359812&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