Glutaric acid, 2,6-dimethylnon-1-en-3-yn-5-yl pentadecyl ester

Inchi: InChI=1S/C31H54O4/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-26-34-30(32)22-20-23-31

InchiKey: SRTRKZQZORUMKW-UHFFFAOYSA-N

Formula: C31H54O4

SMILES: C=C(C)C#CC(OC(=O)CCCC(=O)OCCCCCCCCCCCCCCC)C(C)CCC

Mol. weight [g/mol]: 490.76

Physical Properties

Property code	Value	Unit	Source
gf	19.51	kJ/mol	Joback Method
hf	-795.39	kJ/mol	Joback Method
hfus	75.11	kJ/mol	Joback Method
hvap	103.70	kJ/mol	Joback Method
log10ws	-10.04		Crippen Method
logp	8.719		Crippen Method
mcvol	449.630	ml/mol	McGowan Method
pc	664.60	kPa	Joback Method
rinpol	3259.00		NIST Webbook
rinpol	3259.00		NIST Webbook
tb	1065.94	K	Joback Method
tc	1321.98	K	Joback Method
tf	643.83	K	Joback Method
vc	1.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1581.92	J/mol×K	1065.94	Joback Method
cpg	1603.03	J/mol×K	1108.61	Joback Method
cpg	1621.99	J/mol×K	1151.29	Joback Method
cpg	1638.93	J/mol×K	1193.96	Joback Method
cpg	1653.94	J/mol×K	1236.63	Joback Method
cpg	1667.12	J/mol×K	1279.31	Joback Method
cpg	1678.60	J/mol×K	1321.98	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=U359832&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