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

Inchi: InChI=1S/C32H56O4/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-20-27-35-31(33)23-21-24
InchiKey: HLABGACXUXCARQ-UHFFFAOYSA-N
Formula: C32H56O4
SMILES: C=C(C)C#CC(OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCC)C(C)CCC
Mol. weight [g/mol]: 504.78

Physical Properties

Property code	Value	Unit	Source
gf	27.93	kJ/mol	Joback Method
hf	-816.03	kJ/mol	Joback Method
hfus	77.70	kJ/mol	Joback Method
hvap	105.92	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	9.109		Crippen Method
mcvol	463.720	ml/mol	McGowan Method
pc	632.89	kPa	Joback Method
rinpol	3365.00		NIST Webbook
rinpol	3365.00		NIST Webbook
tb	1088.82	K	Joback Method
tc	1357.47	K	Joback Method
tf	655.10	K	Joback Method
vc	1.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1646.91	J/mol×K	1088.82	Joback Method
cpg	1668.59	J/mol×K	1133.60	Joback Method
cpg	1687.94	J/mol×K	1178.37	Joback Method
cpg	1705.07	J/mol×K	1223.15	Joback Method
cpg	1720.12	J/mol×K	1267.92	Joback Method
cpg	1733.22	J/mol×K	1312.70	Joback Method
cpg	1744.49	J/mol×K	1357.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359833&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