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

Inchi: InChI=1S/C30H54O4/c1-4-7-9-11-12-13-14-15-16-17-18-19-20-22-27-33-29(31)25-23-26
InchiKey: KSNHDEYPHDZEPD-UHFFFAOYSA-N
Formula: C30H54O4
SMILES: CCCC#CCC(CC)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 478.75

Physical Properties

Property code	Value	Unit	Source
gf	-65.76	kJ/mol	Joback Method
hf	-885.11	kJ/mol	Joback Method
hfus	78.63	kJ/mol	Joback Method
hvap	102.45	kJ/mol	Joback Method
log10ws	-10.01		Crippen Method
logp	8.697		Crippen Method
mcvol	439.840	ml/mol	McGowan Method
pc	678.88	kPa	Joback Method
rinpol	3338.00		NIST Webbook
rinpol	3338.00		NIST Webbook
tb	1046.94	K	Joback Method
tc	1299.49	K	Joback Method
tf	663.28	K	Joback Method
vc	1.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.11	J/mol×K	1046.94	Joback Method
cpg	1569.55	J/mol×K	1089.03	Joback Method
cpg	1588.80	J/mol×K	1131.12	Joback Method
cpg	1605.95	J/mol×K	1173.21	Joback Method
cpg	1621.09	J/mol×K	1215.31	Joback Method
cpg	1634.30	J/mol×K	1257.40	Joback Method
cpg	1645.68	J/mol×K	1299.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359813&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

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