Glutaric acid, hexadecyl 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C30H54O4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-25-33-29(31)23-21-24
InchiKey: LRNSQMUZMFZLEF-UHFFFAOYSA-N
Formula: C30H54O4
SMILES: CCC#CC(CC(C)C)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 478.75

Physical Properties

Property code	Value	Unit	Source
gf	-68.20	kJ/mol	Joback Method
hf	-890.39	kJ/mol	Joback Method
hfus	75.11	kJ/mol	Joback Method
hvap	102.06	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.553		Crippen Method
mcvol	439.840	ml/mol	McGowan Method
pc	681.71	kPa	Joback Method
rinpol	3836.00		NIST Webbook
rinpol	3836.00		NIST Webbook
tb	1046.50	K	Joback Method
tc	1296.55	K	Joback Method
tf	648.28	K	Joback Method
vc	1.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.31	J/mol×K	1046.50	Joback Method
cpg	1569.46	J/mol×K	1088.17	Joback Method
cpg	1588.45	J/mol×K	1129.85	Joback Method
cpg	1605.36	J/mol×K	1171.52	Joback Method
cpg	1620.27	J/mol×K	1213.20	Joback Method
cpg	1633.28	J/mol×K	1254.87	Joback Method
cpg	1644.47	J/mol×K	1296.55	Joback Method

Sources

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=U359613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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