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

Inchi: InChI=1S/C31H56O4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-26-34-30(32)24-22

InchiKey: LYUYDTPEFZMIGG-UHFFFAOYSA-N

Formula: C31H56O4

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

Mol. weight [g/mol]: 492.77

Physical Properties

Property code	Value	Unit	Source
gf	-59.78	kJ/mol	Joback Method
hf	-911.03	kJ/mol	Joback Method
hfus	77.70	kJ/mol	Joback Method
hvap	104.29	kJ/mol	Joback Method
log10ws	-10.19		Crippen Method
logp	8.943		Crippen Method
mcvol	453.930	ml/mol	McGowan Method
pc	648.78	kPa	Joback Method
rinpol	3913.00		NIST Webbook
rinpol	3913.00		NIST Webbook
tb	1069.38	K	Joback Method
tc	1331.61	K	Joback Method
tf	659.55	K	Joback Method
vc	1.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1613.22	J/mol×K	1069.38	Joback Method
cpg	1634.91	J/mol×K	1113.09	Joback Method
cpg	1654.22	J/mol×K	1156.79	Joback Method
cpg	1671.26	J/mol×K	1200.50	Joback Method
cpg	1686.13	J/mol×K	1244.20	Joback Method
cpg	1698.92	J/mol×K	1287.91	Joback Method
cpg	1709.76	J/mol×K	1331.61	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=U359614&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

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