Glutaric acid, di(2,6-dimethylnon-1-en-3-yn-5-yl) ester

Inchi: InChI=1S/C27H40O4/c1-9-12-22(7)24(18-16-20(3)4)30-26(28)14-11-15-27(29)31-25(19-

InchiKey: YANURNHVAISHPM-UHFFFAOYSA-N

Formula: C27H40O4

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

Mol. weight [g/mol]: 428.60

Physical Properties

Property code	Value	Unit	Source
gf	263.04	kJ/mol	Joback Method
hf	-335.45	kJ/mol	Joback Method
hfus	58.23	kJ/mol	Joback Method
hvap	95.58	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.012		Crippen Method
mcvol	380.370	ml/mol	McGowan Method
pc	934.06	kPa	Joback Method
rinpol	2607.00		NIST Webbook
rinpol	2607.00		NIST Webbook
tb	979.10	K	Joback Method
tc	1200.64	K	Joback Method
tf	659.13	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.58	J/mol×K	979.10	Joback Method
cpg	1257.09	J/mol×K	1016.02	Joback Method
cpg	1273.17	J/mol×K	1052.95	Joback Method
cpg	1287.87	J/mol×K	1089.87	Joback Method
cpg	1301.24	J/mol×K	1126.79	Joback Method
cpg	1313.34	J/mol×K	1163.72	Joback Method
cpg	1324.22	J/mol×K	1200.64	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=U359834&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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