Glutaric acid, di(2,7-dimethyloct-5-yn-7-en-4-yl) ester

Inchi: InChI=1S/C25H36O4/c1-18(2)12-14-22(16-20(5)6)28-24(26)10-9-11-25(27)29-23(17-21(

InchiKey: LLWKXBOEWFLNHR-UHFFFAOYSA-N

Formula: C25H36O4

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

Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	246.20	kJ/mol	Joback Method
hf	-294.17	kJ/mol	Joback Method
hfus	53.05	kJ/mol	Joback Method
hvap	91.13	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	5.231		Crippen Method
mcvol	352.190	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	2443.00		NIST Webbook
tb	933.34	K	Joback Method
tc	1150.42	K	Joback Method
tf	636.59	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1115.71	J/mol×K	933.34	Joback Method
cpg	1132.98	J/mol×K	969.52	Joback Method
cpg	1148.91	J/mol×K	1005.70	Joback Method
cpg	1163.54	J/mol×K	1041.88	Joback Method
cpg	1176.93	J/mol×K	1078.06	Joback Method
cpg	1189.11	J/mol×K	1114.24	Joback Method
cpg	1200.12	J/mol×K	1150.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359851&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