Glutaric acid, 2,7-dimethyloct-5-yn-7-en-4-yl isohexyl ester

Inchi: InChI=1S/C21H34O4/c1-16(2)9-8-14-24-20(22)10-7-11-21(23)25-19(15-18(5)6)13-12-17

InchiKey: XHXJEMQTYMEMHY-UHFFFAOYSA-N

Formula: C21H34O4

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

Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-67.13	kJ/mol	Joback Method
hf	-594.27	kJ/mol	Joback Method
hfus	45.68	kJ/mol	Joback Method
hvap	81.05	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.674		Crippen Method
mcvol	308.730	ml/mol	McGowan Method
pc	1180.09	kPa	Joback Method
rinpol	2232.00		NIST Webbook
tb	836.70	K	Joback Method
tc	1035.53	K	Joback Method
tf	516.13	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.60	J/mol×K	836.70	Joback Method
cpg	971.20	J/mol×K	869.84	Joback Method
cpg	987.66	J/mol×K	902.98	Joback Method
cpg	1002.99	J/mol×K	936.12	Joback Method
cpg	1017.24	J/mol×K	969.26	Joback Method
cpg	1030.40	J/mol×K	1002.39	Joback Method
cpg	1042.52	J/mol×K	1035.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359839&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