Glutaric acid, 2-methylpent-3-yl 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C22H36O4/c1-8-11-18(7)20(15-14-16(3)4)26-22(24)13-10-12-21(23)25-19(9-2

InchiKey: KNEXJLNFHAWLBX-UHFFFAOYSA-N

Formula: C22H36O4

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

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-61.15	kJ/mol	Joback Method
hf	-620.19	kJ/mol	Joback Method
hfus	44.75	kJ/mol	Joback Method
hvap	82.89	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.062		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2171.00		NIST Webbook
tb	859.14	K	Joback Method
tc	1060.62	K	Joback Method
tf	512.40	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.47	J/mol×K	859.14	Joback Method
cpg	1032.39	J/mol×K	892.72	Joback Method
cpg	1049.10	J/mol×K	926.30	Joback Method
cpg	1064.61	J/mol×K	959.88	Joback Method
cpg	1078.96	J/mol×K	993.46	Joback Method
cpg	1092.17	J/mol×K	1027.04	Joback Method
cpg	1104.26	J/mol×K	1060.62	Joback Method

Sources

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=U393964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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