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

Inchi: InChI=1S/C21H34O4/c1-8-10-17(6)19(14-13-15(2)3)25-21(23)12-9-11-20(22)24-18(7)16

InchiKey: RXPZONYCZAXTJI-UHFFFAOYSA-N

Formula: C21H34O4

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

Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-69.57	kJ/mol	Joback Method
hf	-599.55	kJ/mol	Joback Method
hfus	42.16	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.672		Crippen Method
mcvol	308.730	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook
tb	836.26	K	Joback Method
tc	1036.82	K	Joback Method
tf	501.13	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.09	J/mol×K	836.26	Joback Method
cpg	971.84	J/mol×K	869.69	Joback Method
cpg	988.41	J/mol×K	903.11	Joback Method
cpg	1003.83	J/mol×K	936.54	Joback Method
cpg	1018.12	J/mol×K	969.96	Joback Method
cpg	1031.31	J/mol×K	1003.39	Joback Method
cpg	1043.43	J/mol×K	1036.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393963&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