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

Inchi: InChI=1S/C23H36O4/c1-5-10-19(4)21(16-15-18(2)3)27-23(25)14-9-13-22(24)26-17-20-11-7-6-8-12-20/h5,15-16,18-21H,6-14,17H2,1-4H3/b16-15+

InchiKey: FYUYZFQOPKBZRK-UHFFFAOYSA-N

Formula: C23H36O4

SMILES: C=C(C)C#CC(OC(=O)CCCC(=O)OCC1CCCCC1)C(C)CCC

Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-23.40	kJ/mol	Joback Method
hf	-575.95	kJ/mol	Joback Method
hfus	46.22	kJ/mol	Joback Method
hvap	86.32	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.208		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1184.16	kPa	Joback Method
rinpol	2486.00		NIST Webbook
rinpol	2486.00		NIST Webbook
tb	902.45	K	Joback Method
tc	1117.25	K	Joback Method
tf	561.05	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.90	J/mol×K	902.45	Joback Method
cpg	1089.19	J/mol×K	938.25	Joback Method
cpg	1105.97	J/mol×K	974.05	Joback Method
cpg	1121.27	J/mol×K	1009.85	Joback Method
cpg	1135.14	J/mol×K	1045.65	Joback Method
cpg	1147.62	J/mol×K	1081.45	Joback Method
cpg	1158.74	J/mol×K	1117.25	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=U393967&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