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

Inchi: InChI=1S/C23H38O4/c1-6-8-9-10-11-18-26-22(24)14-12-15-23(25)27-21(17-16-19(3)4)2

InchiKey: NOERFMGTSZMRDW-UHFFFAOYSA-N

Formula: C23H38O4

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

Mol. weight [g/mol]: 378.55

Physical Properties

Property code	Value	Unit	Source
gf	-47.85	kJ/mol	Joback Method
hf	-630.27	kJ/mol	Joback Method
hfus	54.39	kJ/mol	Joback Method
hvap	85.89	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.598		Crippen Method
mcvol	336.910	ml/mol	McGowan Method
pc	1033.24	kPa	Joback Method
rinpol	2450.00		NIST Webbook
tb	882.90	K	Joback Method
tc	1084.08	K	Joback Method
tf	553.67	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.62	J/mol×K	882.90	Joback Method
cpg	1092.59	J/mol×K	916.43	Joback Method
cpg	1109.34	J/mol×K	949.96	Joback Method
cpg	1124.90	J/mol×K	983.49	Joback Method
cpg	1139.29	J/mol×K	1017.02	Joback Method
cpg	1152.55	J/mol×K	1050.55	Joback Method
cpg	1164.70	J/mol×K	1084.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359824&Units=SI

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