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

Inchi: InChI=1S/C22H36O4/c1-6-8-9-10-17-25-21(23)13-11-14-22(24)26-20(16-15-18(3)4)19(5
InchiKey: GPXPZMOEWWUATR-UHFFFAOYSA-N
Formula: C22H36O4
SMILES: C=C(C)C#CC(OC(=O)CCCC(=O)OCCCCCC)C(C)CCC
Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-56.27	kJ/mol	Joback Method
hf	-609.63	kJ/mol	Joback Method
hfus	51.80	kJ/mol	Joback Method
hvap	83.66	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.208		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	2353.00		NIST Webbook
tb	860.02	K	Joback Method
tc	1058.85	K	Joback Method
tf	542.40	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.51	J/mol×K	860.02	Joback Method
cpg	1031.22	J/mol×K	893.16	Joback Method
cpg	1047.78	J/mol×K	926.30	Joback Method
cpg	1063.19	J/mol×K	959.43	Joback Method
cpg	1077.49	J/mol×K	992.57	Joback Method
cpg	1090.69	J/mol×K	1025.71	Joback Method
cpg	1102.84	J/mol×K	1058.85	Joback Method

Sources

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=U359823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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