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

Inchi: InChI=1S/C22H36O4/c1-7-10-19(6)20(15-14-18(4)5)26-22(24)13-8-12-21(23)25-16-9-11

InchiKey: CENUYXVVEASSHW-UHFFFAOYSA-N

Formula: C22H36O4

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

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-58.71	kJ/mol	Joback Method
hf	-614.91	kJ/mol	Joback Method
hfus	48.27	kJ/mol	Joback Method
hvap	83.28	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.064		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	859.58	K	Joback Method
tc	1059.66	K	Joback Method
tf	527.40	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.99	J/mol×K	859.58	Joback Method
cpg	1031.80	J/mol×K	892.93	Joback Method
cpg	1048.42	J/mol×K	926.27	Joback Method
cpg	1063.88	J/mol×K	959.62	Joback Method
cpg	1078.20	J/mol×K	992.97	Joback Method
cpg	1091.41	J/mol×K	1026.32	Joback Method
cpg	1103.53	J/mol×K	1059.66	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=U359822&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