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

Inchi: InChI=1S/C24H40O4/c1-7-10-13-21(9-3)18-27-23(25)14-11-15-24(26)28-22(17-16-19(4)

InchiKey: TYHBDRKGLMFQSE-UHFFFAOYSA-N

Formula: C24H40O4

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

Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	-41.87	kJ/mol	Joback Method
hf	-656.19	kJ/mol	Joback Method
hfus	53.45	kJ/mol	Joback Method
hvap	87.73	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.844		Crippen Method
mcvol	351.000	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	905.34	K	Joback Method
tc	1110.27	K	Joback Method
tf	549.94	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.81	J/mol×K	905.34	Joback Method
cpg	1155.08	J/mol×K	939.50	Joback Method
cpg	1172.05	J/mol×K	973.65	Joback Method
cpg	1187.74	J/mol×K	1007.81	Joback Method
cpg	1202.19	J/mol×K	1041.96	Joback Method
cpg	1215.43	J/mol×K	1076.12	Joback Method
cpg	1227.50	J/mol×K	1110.27	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=U393966&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