Glutaric acid, cyclohexylmethyl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C24H40O4/c1-2-3-4-5-6-7-8-9-10-14-20-27-23(25)18-15-19-24(26)28-21-22-16
InchiKey: RUIKQVFUSCDCQN-UHFFFAOYSA-N
Formula: C24H40O4
SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	-89.39	kJ/mol	Joback Method
hf	-701.67	kJ/mol	Joback Method
hfus	58.45	kJ/mol	Joback Method
hvap	89.91	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.967		Crippen Method
mcvol	344.440	ml/mol	McGowan Method
pc	1064.48	kPa	Joback Method
rinpol	2927.00		NIST Webbook
rinpol	2927.00		NIST Webbook
tb	929.65	K	Joback Method
tc	1141.23	K	Joback Method
tf	618.04	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.30	J/mol×K	929.65	Joback Method
cpg	1179.71	J/mol×K	964.91	Joback Method
cpg	1196.58	J/mol×K	1000.18	Joback Method
cpg	1211.95	J/mol×K	1035.44	Joback Method
cpg	1225.84	J/mol×K	1070.70	Joback Method
cpg	1238.30	J/mol×K	1105.96	Joback Method
cpg	1249.36	J/mol×K	1141.23	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=U393945&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