Glutaric acid, oct-1-en-3-yl hex-4-yn-3-yl ester

Inchi: InChI=1S/C19H30O4/c1-5-9-10-13-17(8-4)23-19(21)15-11-14-18(20)22-16(7-3)12-6-2/h8
InchiKey: SZYOPPTUJHLDCK-UHFFFAOYSA-N
Formula: C19H30O4
SMILES: C=CC(CCCCC)OC(=O)CCCC(=O)OC(C#CC)CC
Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-72.98	kJ/mol	Joback Method
hf	-537.92	kJ/mol	Joback Method
hfus	45.34	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.180		Crippen Method
mcvol	280.550	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	791.50	K	Joback Method
tc	985.94	K	Joback Method
tf	522.55	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.04	J/mol×K	791.50	Joback Method
cpg	851.88	J/mol×K	823.91	Joback Method
cpg	867.70	J/mol×K	856.31	Joback Method
cpg	882.52	J/mol×K	888.72	Joback Method
cpg	896.35	J/mol×K	921.13	Joback Method
cpg	909.23	J/mol×K	953.53	Joback Method
cpg	921.15	J/mol×K	985.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405349&Units=SI
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

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