Glutaric acid, but-3-en-2-yl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C22H36O4/c1-4-6-7-8-9-10-11-12-13-14-15-19-25-21(23)17-16-18-22(24)26-2
InchiKey: XEBGSGRRGLVUEH-UHFFFAOYSA-N
Formula: C22H36O4
SMILES: C=CC(C)OC(=O)CCCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-45.28	kJ/mol	Joback Method
hf	-594.56	kJ/mol	Joback Method
hfus	56.63	kJ/mol	Joback Method
hvap	83.97	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.352		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1090.66	kPa	Joback Method
rinpol	2491.00		NIST Webbook
rinpol	2491.00		NIST Webbook
tb	860.58	K	Joback Method
tc	1057.42	K	Joback Method
tf	571.36	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.41	J/mol×K	860.58	Joback Method
cpg	1030.96	J/mol×K	893.39	Joback Method
cpg	1047.38	J/mol×K	926.19	Joback Method
cpg	1062.68	J/mol×K	959.00	Joback Method
cpg	1076.89	J/mol×K	991.81	Joback Method
cpg	1090.04	J/mol×K	1024.62	Joback Method
cpg	1102.15	J/mol×K	1057.42	Joback Method

Sources

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=U405248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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