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

Inchi: InChI=1S/C22H34O4/c1-4-6-7-8-9-10-11-12-13-14-15-19-25-21(23)17-16-18-22(24)26-2
InchiKey: TUNRMAFEKIQDNW-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	89.95	kJ/mol	Joback Method
hf	-428.09	kJ/mol	Joback Method
hfus	60.88	kJ/mol	Joback Method
hvap	84.50	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	4.799		Crippen Method
mcvol	318.520	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2487.00		NIST Webbook
rinpol	2487.00		NIST Webbook
tb	854.02	K	Joback Method
tc	1052.60	K	Joback Method
tf	620.09	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.70	J/mol×K	854.02	Joback Method
cpg	1000.82	J/mol×K	887.12	Joback Method
cpg	1016.84	J/mol×K	920.21	Joback Method
cpg	1031.79	J/mol×K	953.31	Joback Method
cpg	1045.69	J/mol×K	986.41	Joback Method
cpg	1058.57	J/mol×K	1019.50	Joback Method
cpg	1070.45	J/mol×K	1052.60	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=U394008&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