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

Inchi: InChI=1S/C21H34O4/c1-4-6-7-8-9-10-11-12-13-14-18-24-20(22)16-15-17-21(23)25-19(3
InchiKey: VPYIHOYMMCFEAZ-BUHFOSPRSA-N
Formula: C21H34O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCC=CCCCCCCCCC
Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-41.05	kJ/mol	Joback Method
hf	-562.53	kJ/mol	Joback Method
hfus	55.37	kJ/mol	Joback Method
hvap	80.08	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.962		Crippen Method
mcvol	308.730	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	2352.00		NIST Webbook
rinpol	2352.00		NIST Webbook
tb	826.30	K	Joback Method
tc	1017.91	K	Joback Method
tf	497.64	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.38	J/mol×K	826.30	Joback Method
cpg	965.52	J/mol×K	858.23	Joback Method
cpg	981.66	J/mol×K	890.17	Joback Method
cpg	996.84	J/mol×K	922.10	Joback Method
cpg	1011.09	J/mol×K	954.04	Joback Method
cpg	1024.46	J/mol×K	985.97	Joback Method
cpg	1036.96	J/mol×K	1017.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394007&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

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