Glutaric acid, but-3-en-2-yl hex-4-yn-3-yl ester

Inchi: InChI=1S/C15H22O4/c1-5-9-13(7-3)19-15(17)11-8-10-14(16)18-12(4)6-2/h6,12-13H,2,7-
InchiKey: CEBIILHLXWTOOK-UHFFFAOYSA-N
Formula: C15H22O4
SMILES: C=CC(C)OC(=O)CCCC(=O)OC(C#CC)CC
Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-106.66	kJ/mol	Joback Method
hf	-455.36	kJ/mol	Joback Method
hfus	34.98	kJ/mol	Joback Method
hvap	68.00	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.619		Crippen Method
mcvol	224.190	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	699.98	K	Joback Method
tc	898.37	K	Joback Method
tf	477.47	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.81	J/mol×K	699.98	Joback Method
cpg	625.32	J/mol×K	733.04	Joback Method
cpg	639.96	J/mol×K	766.11	Joback Method
cpg	653.75	J/mol×K	799.17	Joback Method
cpg	666.70	J/mol×K	832.24	Joback Method
cpg	678.82	J/mol×K	865.30	Joback Method
cpg	690.10	J/mol×K	898.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405236&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