Glutaric acid, but-3-yn-2-yl oct-3-en-2-yl ester

Inchi: InChI=1S/C17H26O4/c1-5-7-8-9-11-15(4)21-17(19)13-10-12-16(18)20-14(3)6-2/h2,9,11,1
InchiKey: ZKOPAMBUVNBPHW-PKNBQFBNSA-N
Formula: C17H26O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OC(C)C=CCCCC
Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
gf	-77.17	kJ/mol	Joback Method
hf	-485.25	kJ/mol	Joback Method
hfus	41.49	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.400		Crippen Method
mcvol	252.370	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1868.00		NIST Webbook
rinpol	1868.00		NIST Webbook
tb	734.34	K	Joback Method
tc	925.89	K	Joback Method
tf	437.56	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.97	J/mol×K	734.34	Joback Method
cpg	732.90	J/mol×K	766.26	Joback Method
cpg	747.94	J/mol×K	798.19	Joback Method
cpg	762.13	J/mol×K	830.11	Joback Method
cpg	775.48	J/mol×K	862.04	Joback Method
cpg	788.03	J/mol×K	893.96	Joback Method
cpg	799.79	J/mol×K	925.89	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=U393984&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

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