Glutaric acid, but-3-yn-2-yl 2-methylpent-3-yl ester

Inchi: InChI=1S/C15H24O4/c1-6-12(5)18-14(16)9-8-10-15(17)19-13(7-2)11(3)4/h1,11-13H,7-10
InchiKey: VSZWYAFERJODPA-UHFFFAOYSA-N
Formula: C15H24O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-176.67	kJ/mol	Joback Method
hf	-566.47	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.699		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1644.00		NIST Webbook
rinpol	1644.00		NIST Webbook
tb	683.98	K	Joback Method
tc	874.84	K	Joback Method
tf	405.10	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.39	J/mol×K	683.98	Joback Method
cpg	646.29	J/mol×K	715.79	Joback Method
cpg	661.34	J/mol×K	747.60	Joback Method
cpg	675.56	J/mol×K	779.41	Joback Method
cpg	688.96	J/mol×K	811.22	Joback Method
cpg	701.55	J/mol×K	843.03	Joback Method
cpg	713.34	J/mol×K	874.84	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=U393492&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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