Glutaric acid, but-3-yn-2-yl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C16H26O4/c1-7-13(6)19-14(17)9-8-10-15(18)20-16(11(2)3)12(4)5/h1,11-13,16

InchiKey: YBMUHHBBHBAOLK-UHFFFAOYSA-N

Formula: C16H26O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-170.69	kJ/mol	Joback Method
hf	-592.39	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	67.83	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.945		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	1695.00		NIST Webbook
rinpol	1695.00		NIST Webbook
tb	706.42	K	Joback Method
tc	898.71	K	Joback Method
tf	401.37	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.67	J/mol×K	706.42	Joback Method
cpg	702.22	J/mol×K	738.47	Joback Method
cpg	717.86	J/mol×K	770.52	Joback Method
cpg	732.59	J/mol×K	802.56	Joback Method
cpg	746.44	J/mol×K	834.61	Joback Method
cpg	759.41	J/mol×K	866.66	Joback Method
cpg	771.53	J/mol×K	898.71	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=U393472&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