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

Inchi: InChI=1S/C14H20O4/c1-5-12(4)18-14(16)8-6-7-13(15)17-10-9-11(2)3/h1,9,12H,6-8,10H2

InchiKey: FNRIPHJBAOFELT-UHFFFAOYSA-N

Formula: C14H20O4

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

Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	-108.54	kJ/mol	Joback Method
hf	-427.84	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	64.58	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.231		Crippen Method
mcvol	210.100	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
tb	666.02	K	Joback Method
tc	861.60	K	Joback Method
tf	404.79	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.64	J/mol×K	666.02	Joback Method
cpg	568.20	J/mol×K	698.62	Joback Method
cpg	581.98	J/mol×K	731.21	Joback Method
cpg	595.01	J/mol×K	763.81	Joback Method
cpg	607.30	J/mol×K	796.41	Joback Method
cpg	618.88	J/mol×K	829.01	Joback Method
cpg	629.76	J/mol×K	861.60	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=U393994&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