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

Inchi: InChI=1S/C14H22O4/c1-6-11(2)18-13(16)9-7-8-12(15)17-10-14(3,4)5/h1,11H,7-10H2,2-5
InchiKey: PLRVDVXBZFJZGV-UHFFFAOYSA-N
Formula: C14H22O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-177.37	kJ/mol	Joback Method
hf	-544.02	kJ/mol	Joback Method
hfus	29.63	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.311		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
tb	658.75	K	Joback Method
tc	853.97	K	Joback Method
tf	426.25	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.76	J/mol×K	658.75	Joback Method
cpg	594.16	J/mol×K	691.29	Joback Method
cpg	608.70	J/mol×K	723.82	Joback Method
cpg	622.41	J/mol×K	756.36	Joback Method
cpg	635.30	J/mol×K	788.90	Joback Method
cpg	647.41	J/mol×K	821.44	Joback Method
cpg	658.76	J/mol×K	853.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391606&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

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