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

Inchi: InChI=1S/C16H22O4/c1-3-11(2)19-15(17)5-4-6-16(18)20-14-10-12-7-8-13(14)9-12/h1,11
InchiKey: MZSQLNDULFIOJH-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OC1CC2CCC1C2
Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-61.68	kJ/mol	Joback Method
hf	-457.45	kJ/mol	Joback Method
hfus	37.46	kJ/mol	Joback Method
hvap	68.68	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.453		Crippen Method
mcvol	220.860	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1924.00		NIST Webbook
rinpol	1924.00		NIST Webbook
tb	720.82	K	Joback Method
tc	930.06	K	Joback Method
tf	474.49	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.55	J/mol×K	720.82	Joback Method
cpg	676.87	J/mol×K	755.69	Joback Method
cpg	693.10	J/mol×K	790.57	Joback Method
cpg	708.29	J/mol×K	825.44	Joback Method
cpg	722.50	J/mol×K	860.31	Joback Method
cpg	735.77	J/mol×K	895.19	Joback Method
cpg	748.17	J/mol×K	930.06	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=U405485&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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