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

Inchi: InChI=1S/C16H24O4/c1-3-13(2)20-16(18)11-7-10-15(17)19-12-14-8-5-4-6-9-14/h1,13-14

InchiKey: KKZPHWTYLLKRPI-UHFFFAOYSA-N

Formula: C16H24O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-138.92	kJ/mol	Joback Method
hf	-522.23	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	69.42	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.845		Crippen Method
mcvol	231.720	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	727.29	K	Joback Method
tc	936.21	K	Joback Method
tf	453.75	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.37	J/mol×K	727.29	Joback Method
cpg	696.23	J/mol×K	762.11	Joback Method
cpg	712.92	J/mol×K	796.93	Joback Method
cpg	728.44	J/mol×K	831.75	Joback Method
cpg	742.83	J/mol×K	866.57	Joback Method
cpg	756.09	J/mol×K	901.39	Joback Method
cpg	768.26	J/mol×K	936.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394000&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