Glutaric acid, (cyclohex-3-enyl)methyl but-3-yn-2-yl ester

Inchi: InChI=1S/C16H22O4/c1-3-13(2)20-16(18)11-7-10-15(17)19-12-14-8-5-4-6-9-14/h1,4-5,1

InchiKey: QOVYIWVTBVQXSH-UHFFFAOYSA-N

Formula: C16H22O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OCC1CC=CCC1

Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-108.96	kJ/mol	Joback Method
hf	-464.45	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	69.71	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.621		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
tb	726.45	K	Joback Method
tc	936.88	K	Joback Method
tf	454.51	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.34	J/mol×K	726.45	Joback Method
cpg	670.31	J/mol×K	761.52	Joback Method
cpg	686.13	J/mol×K	796.59	Joback Method
cpg	700.83	J/mol×K	831.66	Joback Method
cpg	714.43	J/mol×K	866.74	Joback Method
cpg	726.95	J/mol×K	901.81	Joback Method
cpg	738.41	J/mol×K	936.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405523&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

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