Glutaric acid, (2-methylcyclohex-1-enyl)methyl but-3-yn-2-yl ester

Inchi: InChI=1S/C17H24O4/c1-4-14(3)21-17(19)11-7-10-16(18)20-12-15-9-6-5-8-13(15)2/h1,14
InchiKey: XPIZRAMMSOBATK-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCC1=C(C)CCCC1
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-112.09	kJ/mol	Joback Method
hf	-487.69	kJ/mol	Joback Method
hfus	36.02	kJ/mol	Joback Method
hvap	73.57	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.155		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2005.00		NIST Webbook
rinpol	2005.00		NIST Webbook
tb	763.96	K	Joback Method
tc	973.67	K	Joback Method
tf	495.06	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.96	J/mol×K	763.96	Joback Method
cpg	721.45	J/mol×K	798.91	Joback Method
cpg	736.82	J/mol×K	833.86	Joback Method
cpg	751.10	J/mol×K	868.81	Joback Method
cpg	764.31	J/mol×K	903.76	Joback Method
cpg	776.47	J/mol×K	938.72	Joback Method
cpg	787.59	J/mol×K	973.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405501&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