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

Inchi: InChI=1S/C15H24O4/c1-5-13(4)19-15(17)10-6-9-14(16)18-11-7-8-12(2)3/h1,12-13H,6-11
InchiKey: ODFVLBINMDSXIJ-UHFFFAOYSA-N
Formula: C15H24O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-174.23	kJ/mol	Joback Method
hf	-561.19	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.701		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1778.00		NIST Webbook
tb	684.42	K	Joback Method
tc	872.41	K	Joback Method
tf	420.10	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.90	J/mol×K	684.42	Joback Method
cpg	645.54	J/mol×K	715.75	Joback Method
cpg	660.36	J/mol×K	747.08	Joback Method
cpg	674.38	J/mol×K	778.42	Joback Method
cpg	687.61	J/mol×K	809.75	Joback Method
cpg	700.07	J/mol×K	841.08	Joback Method
cpg	711.75	J/mol×K	872.41	Joback Method

Sources

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=U359876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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