Glutaric acid, hex-4-yn-3-yl propyl ester

Inchi: InChI=1S/C14H22O4/c1-4-8-12(6-3)18-14(16)10-7-9-13(15)17-11-5-2/h12H,5-7,9-11H2,1
InchiKey: FNGIVOGZPOXAIM-UHFFFAOYSA-N
Formula: C14H22O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCC
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-200.48	kJ/mol	Joback Method
hf	-554.87	kJ/mol	Joback Method
hfus	37.19	kJ/mol	Joback Method
hvap	66.83	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.455		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1770.00		NIST Webbook
tb	680.86	K	Joback Method
tc	875.06	K	Joback Method
tf	482.96	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.18	J/mol×K	680.86	Joback Method
cpg	594.51	J/mol×K	713.23	Joback Method
cpg	609.05	J/mol×K	745.59	Joback Method
cpg	622.81	J/mol×K	777.96	Joback Method
cpg	635.78	J/mol×K	810.32	Joback Method
cpg	647.96	J/mol×K	842.69	Joback Method
cpg	659.36	J/mol×K	875.06	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=U359853&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