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

Inchi: InChI=1S/C13H20O4/c1-4-8-11(5-2)17-13(15)10-7-9-12(14)16-6-3/h11H,5-7,9-10H2,1-3
InchiKey: QZNNXROZCXVZBK-UHFFFAOYSA-N
Formula: C13H20O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCC
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-208.90	kJ/mol	Joback Method
hf	-534.23	kJ/mol	Joback Method
hfus	34.60	kJ/mol	Joback Method
hvap	64.61	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.065		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1669.00		NIST Webbook
rinpol	1669.00		NIST Webbook
tb	657.98	K	Joback Method
tc	854.21	K	Joback Method
tf	471.69	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.43	J/mol×K	657.98	Joback Method
cpg	541.24	J/mol×K	690.68	Joback Method
cpg	555.31	J/mol×K	723.39	Joback Method
cpg	568.64	J/mol×K	756.09	Joback Method
cpg	581.22	J/mol×K	788.80	Joback Method
cpg	593.06	J/mol×K	821.50	Joback Method
cpg	604.14	J/mol×K	854.21	Joback Method

Sources

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=U359852&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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