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

Inchi: InChI=1S/C17H28O4/c1-4-7-8-9-14-20-16(18)12-10-13-17(19)21-15(6-3)11-5-2/h15H,4,6
InchiKey: SKVUSZAZXGCAQB-UHFFFAOYSA-N
Formula: C17H28O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCCCCC
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-175.22	kJ/mol	Joback Method
hf	-616.79	kJ/mol	Joback Method
hfus	44.96	kJ/mol	Joback Method
hvap	73.51	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.625		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	2063.00		NIST Webbook
tb	749.50	K	Joback Method
tc	940.19	K	Joback Method
tf	516.77	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.99	J/mol×K	749.50	Joback Method
cpg	761.52	J/mol×K	781.28	Joback Method
cpg	777.14	J/mol×K	813.06	Joback Method
cpg	791.84	J/mol×K	844.85	Joback Method
cpg	805.64	J/mol×K	876.63	Joback Method
cpg	818.55	J/mol×K	908.41	Joback Method
cpg	830.58	J/mol×K	940.19	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=U359857&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