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

Inchi: InChI=1S/C17H28O4/c1-5-10-14(7-3)20-16(18)12-9-13-17(19)21-15(8-4)11-6-2/h14-15H
InchiKey: XSFIRLSOJMAYLF-UHFFFAOYSA-N
Formula: C17H28O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OC(CC)CCC
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-177.66	kJ/mol	Joback Method
hf	-622.07	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	73.12	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.624		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	1883.00		NIST Webbook
rinpol	1883.00		NIST Webbook
tb	749.06	K	Joback Method
tc	942.12	K	Joback Method
tf	501.77	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.50	J/mol×K	749.06	Joback Method
cpg	762.25	J/mol×K	781.24	Joback Method
cpg	778.05	J/mol×K	813.41	Joback Method
cpg	792.91	J/mol×K	845.59	Joback Method
cpg	806.83	J/mol×K	877.77	Joback Method
cpg	819.83	J/mol×K	909.94	Joback Method
cpg	831.91	J/mol×K	942.12	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=U393551&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