Glutaric acid, di(hex-4-yn-3-yl) ester

Inchi: InChI=1S/C17H24O4/c1-5-10-14(7-3)20-16(18)12-9-13-17(19)21-15(8-4)11-6-2/h14-15H
InchiKey: QDYORRCHHWXTAI-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OC(C#CC)CC
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	25.14	kJ/mol	Joback Method
hf	-349.77	kJ/mol	Joback Method
hfus	44.56	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	2.847		Crippen Method
mcvol	248.070	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2036.00		NIST Webbook
tb	758.06	K	Joback Method
tc	966.95	K	Joback Method
tf	607.87	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.07	J/mol×K	758.06	Joback Method
cpg	714.30	J/mol×K	792.87	Joback Method
cpg	729.53	J/mol×K	827.69	Joback Method
cpg	743.75	J/mol×K	862.50	Joback Method
cpg	756.98	J/mol×K	897.32	Joback Method
cpg	769.22	J/mol×K	932.13	Joback Method
cpg	780.47	J/mol×K	966.95	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=U359870&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