Glutaric acid, hex-4-yn-3-yl 2-methylphenyl ester

Inchi: InChI=1S/C18H22O4/c1-4-9-15(5-2)21-17(19)12-8-13-18(20)22-16-11-7-6-10-14(16)3/h6
InchiKey: LNEFFUXOFCMHSO-UHFFFAOYSA-N
Formula: C18H22O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccccc1C
Mol. weight [g/mol]: 302.36

Physical Properties

Property code	Value	Unit	Source
gf	-64.02	kJ/mol	Joback Method
hf	-412.37	kJ/mol	Joback Method
hfus	41.20	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.416		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tb	804.04	K	Joback Method
tc	1021.90	K	Joback Method
tf	566.98	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.88	J/mol×K	804.04	Joback Method
cpg	727.14	J/mol×K	840.35	Joback Method
cpg	741.25	J/mol×K	876.66	Joback Method
cpg	754.24	J/mol×K	912.97	Joback Method
cpg	766.11	J/mol×K	949.28	Joback Method
cpg	776.88	J/mol×K	985.59	Joback Method
cpg	786.57	J/mol×K	1021.90	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=U391808&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