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

Inchi: InChI=1S/C19H22O5/c1-4-7-16(5-2)23-18(21)8-6-9-19(22)24-17-12-10-15(11-13-17)14(3
InchiKey: GTJOMMMYQCQVKR-UHFFFAOYSA-N
Formula: C19H22O5
SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 330.38

Physical Properties

Property code	Value	Unit	Source
gf	-184.52	kJ/mol	Joback Method
hf	-545.59	kJ/mol	Joback Method
hfus	45.39	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.310		Crippen Method
mcvol	262.660	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	2555.00		NIST Webbook
rinpol	2555.00		NIST Webbook
tb	880.79	K	Joback Method
tc	1103.02	K	Joback Method
tf	628.18	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.51	J/mol×K	880.79	Joback Method
cpg	795.97	J/mol×K	917.83	Joback Method
cpg	808.20	J/mol×K	954.87	Joback Method
cpg	819.22	J/mol×K	991.90	Joback Method
cpg	829.03	J/mol×K	1028.94	Joback Method
cpg	837.67	J/mol×K	1065.98	Joback Method
cpg	845.15	J/mol×K	1103.02	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=U392034&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