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

Inchi: InChI=1S/C19H24O4/c1-5-9-16(6-2)22-18(20)12-8-13-19(21)23-17-11-7-10-14(3)15(17)4

InchiKey: UQFJBSVQVNQKAC-UHFFFAOYSA-N

Formula: C19H24O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	-65.23	kJ/mol	Joback Method
hf	-444.48	kJ/mol	Joback Method
hfus	43.40	kJ/mol	Joback Method
hvap	81.56	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.724		Crippen Method
mcvol	261.090	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2333.00		NIST Webbook
tb	831.90	K	Joback Method
tc	1048.53	K	Joback Method
tf	590.77	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.89	J/mol×K	831.90	Joback Method
cpg	783.24	J/mol×K	868.00	Joback Method
cpg	797.40	J/mol×K	904.11	Joback Method
cpg	810.40	J/mol×K	940.21	Joback Method
cpg	822.25	J/mol×K	976.32	Joback Method
cpg	832.96	J/mol×K	1012.42	Joback Method
cpg	842.54	J/mol×K	1048.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392219&Units=SI
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

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