Glutaric acid, hex-4-yn-3-yl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C19H24O6/c1-5-9-14(6-2)24-17(20)12-8-13-18(21)25-19-15(22-3)10-7-11-16(1

InchiKey: HIZJIOYKEKCFAT-UHFFFAOYSA-N

Formula: C19H24O6

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 348.39

Physical Properties

Property code	Value	Unit	Source
gf	-275.23	kJ/mol	Joback Method
hf	-708.92	kJ/mol	Joback Method
hfus	45.78	kJ/mol	Joback Method
hvap	86.38	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.125		Crippen Method
mcvol	272.830	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	2503.00		NIST Webbook
tb	876.74	K	Joback Method
tc	1092.44	K	Joback Method
tf	635.23	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.73	J/mol×K	876.74	Joback Method
cpg	837.83	J/mol×K	912.69	Joback Method
cpg	850.58	J/mol×K	948.64	Joback Method
cpg	861.95	J/mol×K	984.59	Joback Method
cpg	871.94	J/mol×K	1020.54	Joback Method
cpg	880.51	J/mol×K	1056.49	Joback Method
cpg	887.66	J/mol×K	1092.44	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=U392003&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