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

Inchi: InChI=1S/C18H22O5/c1-4-9-14(5-2)22-17(19)12-8-13-18(20)23-16-11-7-6-10-15(16)21-3

InchiKey: QSIWSUQHRDYBOB-UHFFFAOYSA-N

Formula: C18H22O5

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccccc1OC

Mol. weight [g/mol]: 318.36

Physical Properties

Property code	Value	Unit	Source
gf	-169.02	kJ/mol	Joback Method
hf	-544.59	kJ/mol	Joback Method
hfus	42.39	kJ/mol	Joback Method
hvap	81.09	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.116		Crippen Method
mcvol	252.870	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2329.00		NIST Webbook
rinpol	2329.00		NIST Webbook
tb	826.46	K	Joback Method
tc	1043.06	K	Joback Method
tf	589.21	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.59	J/mol×K	826.46	Joback Method
cpg	754.31	J/mol×K	862.56	Joback Method
cpg	767.83	J/mol×K	898.66	Joback Method
cpg	780.15	J/mol×K	934.76	Joback Method
cpg	791.26	J/mol×K	970.86	Joback Method
cpg	801.17	J/mol×K	1006.96	Joback Method
cpg	809.88	J/mol×K	1043.06	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=U391758&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