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

Inchi: InChI=1S/C19H24O4/c1-4-10-16(6-3)22-18(20)13-9-14-19(21)23-17-12-8-7-11-15(17)5-2
InchiKey: GPOUKPXKUPTXLN-UHFFFAOYSA-N
Formula: C19H24O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccccc1CC
Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	-55.60	kJ/mol	Joback Method
hf	-433.01	kJ/mol	Joback Method
hfus	43.79	kJ/mol	Joback Method
hvap	80.90	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	3.670		Crippen Method
mcvol	261.090	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2245.00		NIST Webbook
tb	826.92	K	Joback Method
tc	1042.78	K	Joback Method
tf	578.25	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.81	J/mol×K	826.92	Joback Method
cpg	784.24	J/mol×K	862.90	Joback Method
cpg	798.50	J/mol×K	898.87	Joback Method
cpg	811.60	J/mol×K	934.85	Joback Method
cpg	823.57	J/mol×K	970.82	Joback Method
cpg	834.41	J/mol×K	1006.80	Joback Method
cpg	844.15	J/mol×K	1042.78	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=U391472&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