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

Inchi: InChI=1S/C19H32O4/c1-7-10-16(8-2)23-18(21)12-9-11-17(20)22-14-15(3)13-19(4,5)6/h1

InchiKey: AJIFYNWMJRAUMO-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-157.98	kJ/mol	Joback Method
hf	-672.10	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.117		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	791.59	K	Joback Method
tc	990.06	K	Joback Method
tf	526.73	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.80	J/mol×K	791.59	Joback Method
cpg	880.37	J/mol×K	824.67	Joback Method
cpg	896.84	J/mol×K	857.75	Joback Method
cpg	912.26	J/mol×K	890.82	Joback Method
cpg	926.65	J/mol×K	923.90	Joback Method
cpg	940.04	J/mol×K	956.98	Joback Method
cpg	952.47	J/mol×K	990.06	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=U391530&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