Glutaric acid, 3-methylbut-2-yl 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C19H32O4/c1-7-8-10-17(13-14(2)3)23-19(21)12-9-11-18(20)22-16(6)15(4)5/h1
InchiKey: ZBSSYDBKPNLZAS-UHFFFAOYSA-N
Formula: C19H32O4
SMILES: CCC#CC(CC(C)C)OC(=O)CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-165.70	kJ/mol	Joback Method
hf	-673.91	kJ/mol	Joback Method
hfus	39.57	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.116		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
tb	793.94	K	Joback Method
tc	990.72	K	Joback Method
tf	494.31	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.46	J/mol×K	793.94	Joback Method
cpg	880.15	J/mol×K	826.74	Joback Method
cpg	896.73	J/mol×K	859.53	Joback Method
cpg	912.23	J/mol×K	892.33	Joback Method
cpg	926.65	J/mol×K	925.12	Joback Method
cpg	940.01	J/mol×K	957.92	Joback Method
cpg	952.33	J/mol×K	990.72	Joback Method

Sources

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=U394017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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