Glutaric acid, but-3-yn-2-yl 3,7-dimethyloctyl ester

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

InchiKey: HGRGOSXRMFYELP-UHFFFAOYSA-N

Formula: C19H32O4

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

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-142.99	kJ/mol	Joback Method
hf	-649.03	kJ/mol	Joback Method
hfus	42.95	kJ/mol	Joback Method
hvap	74.89	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.117		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	2066.00		NIST Webbook
rinpol	2066.00		NIST Webbook
tb	775.50	K	Joback Method
tc	964.08	K	Joback Method
tf	450.18	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.25	J/mol×K	775.50	Joback Method
cpg	873.52	J/mol×K	806.93	Joback Method
cpg	889.80	J/mol×K	838.36	Joback Method
cpg	905.11	J/mol×K	869.79	Joback Method
cpg	919.45	J/mol×K	901.22	Joback Method
cpg	932.86	J/mol×K	932.65	Joback Method
cpg	945.35	J/mol×K	964.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391482&Units=SI
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

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