

Glutaric acid, but-3-yn-2-yl 2-decyl ester

Inchi: InChI=1S/C19H32O4/c1-5-7-8-9-10-11-13-17(4)23-19(21)15-12-14-18(20)22-16(3)6-2/h2
InchiKey: FOZBKTGOOZTXKM-UHFFFAOYSA-N
Formula: C19H32O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OC(C)CCCCCCCC
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-140.55	kJ/mol	Joback Method
hf	-643.75	kJ/mol	Joback Method
hfus	46.47	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.404		Crippen Method
mvol	284.850	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	2039.00		NIST Webbook
rinpol	2039.00		NIST Webbook
tb	775.94	K	Joback Method
tc	962.74	K	Joback Method
tf	465.18	K	Joback Method
vc	1.097	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.75	J/mol×K	775.94	Joback Method
cpg	872.85	J/mol×K	807.07	Joback Method
cpg	888.99	J/mol×K	838.21	Joback Method
cpg	904.18	J/mol×K	869.34	Joback Method
cpg	918.43	J/mol×K	900.47	Joback Method
cpg	931.78	J/mol×K	931.61	Joback Method
cpg	944.23	J/mol×K	962.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393505&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/89-334-3/Glutaric-acid-but-3-yn-2-yl-2-decyl-ester.pdf>

Generated by Cheméo on 2024-04-20 16:16:31.837374968 +0000 UTC m=+15919040.757952290.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.