Succinic acid, 2-methylpent-3-yl non-5-yn-3-yl ester

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

InchiKey: FLGYOPZISDHYPZ-UHFFFAOYSA-N

Formula: C19H32O4

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

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-163.26	kJ/mol	Joback Method
hf	-668.63	kJ/mol	Joback Method
hfus	43.09	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.260		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		NIST Webbook
tb	794.38	K	Joback Method
tc	989.09	K	Joback Method
tf	509.31	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.96	J/mol×K	794.38	Joback Method
cpg	879.45	J/mol×K	826.83	Joback Method
cpg	895.88	J/mol×K	859.28	Joback Method
cpg	911.26	J/mol×K	891.74	Joback Method
cpg	925.59	J/mol×K	924.19	Joback Method
cpg	938.89	J/mol×K	956.64	Joback Method
cpg	951.18	J/mol×K	989.09	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=U391009&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