Succinic acid, di(2-methyloct-5-yn-4-yl) ester

Inchi: InChI=1S/C22H34O4/c1-7-9-11-19(15-17(3)4)25-21(23)13-14-22(24)26-20(12-10-8-2)16
InchiKey: OJJLYZOWTLWIFX-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCC#CC(CC(C)C)OC(=O)CCC(=O)OC(C#CCC)CC(C)C
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	62.36	kJ/mol	Joback Method
hf	-463.53	kJ/mol	Joback Method
hfus	50.46	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.509		Crippen Method
mcvol	318.520	ml/mol	McGowan Method
pc	1200.62	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	871.58	K	Joback Method
tc	1080.63	K	Joback Method
tf	634.22	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.96	J/mol×K	871.58	Joback Method
cpg	1008.48	J/mol×K	906.42	Joback Method
cpg	1024.73	J/mol×K	941.26	Joback Method
cpg	1039.72	J/mol×K	976.11	Joback Method
cpg	1053.46	J/mol×K	1010.95	Joback Method
cpg	1065.99	J/mol×K	1045.79	Joback Method
cpg	1077.31	J/mol×K	1080.63	Joback Method

Sources

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=U391030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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