Succinic acid, di(2,6-dimethylnon-1-en-3-yn-5-yl) ester

Inchi: InChI=1S/C26H38O4/c1-9-11-21(7)23(15-13-19(3)4)29-25(27)17-18-26(28)30-24(16-14-
InchiKey: QENHXWUDJOXVGS-UHFFFAOYSA-N
Formula: C26H38O4
SMILES: C=C(C)C#CC(OC(=O)CCC(=O)OC(C#CC(=C)C)C(C)CCC)C(C)CCC
Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	254.62	kJ/mol	Joback Method
hf	-314.81	kJ/mol	Joback Method
hfus	55.64	kJ/mol	Joback Method
hvap	93.35	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	5.622		Crippen Method
mcvol	366.280	ml/mol	McGowan Method
pc	991.38	kPa	Joback Method
rinpol	2454.00		NIST Webbook
rinpol	2454.00		NIST Webbook
tb	956.22	K	Joback Method
tc	1175.08	K	Joback Method
tf	647.86	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.39	J/mol×K	956.22	Joback Method
cpg	1194.76	J/mol×K	992.70	Joback Method
cpg	1210.76	J/mol×K	1029.17	Joback Method
cpg	1225.43	J/mol×K	1065.65	Joback Method
cpg	1238.80	J/mol×K	1102.13	Joback Method
cpg	1250.95	J/mol×K	1138.60	Joback Method
cpg	1261.90	J/mol×K	1175.08	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=U391018&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