Succinic acid, 3-methylbut-2-en-1-yl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C21H34O4/c1-4-5-6-7-8-9-10-11-12-13-17-24-20(22)14-15-21(23)25-18-16-19

InchiKey: JKSJLWUAUMMAOI-UHFFFAOYSA-N

Formula: C21H34O4

SMILES: CCC#CCCCCCCCCOC(=O)CCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-67.43	kJ/mol	Joback Method
hf	-586.64	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	82.84	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.963		Crippen Method
mcvol	308.730	ml/mol	McGowan Method
pc	1168.82	kPa	Joback Method
rinpol	2535.00		NIST Webbook
rinpol	2535.00		NIST Webbook
tb	845.50	K	Joback Method
tc	1042.35	K	Joback Method
tf	557.81	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.43	J/mol×K	845.50	Joback Method
cpg	970.69	J/mol×K	878.31	Joback Method
cpg	986.90	J/mol×K	911.12	Joback Method
cpg	1002.10	J/mol×K	943.92	Joback Method
cpg	1016.31	J/mol×K	976.73	Joback Method
cpg	1029.56	J/mol×K	1009.54	Joback Method
cpg	1041.88	J/mol×K	1042.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390997&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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