

Succinic acid, hex-4-yn-3-yl pent-4-en-2-yl ester

Inchi:	InChI=1S/C15H22O4/c1-5-8-12(4)18-14(16)10-11-15(17)19-13(7-3)9-6-2/h5,12-13H,1,7-
InchiKey:	FXVINYCKOQKHNO-UHFFFAOYSA-N
Formula:	C15H22O4
SMILES:	<chem>C=CCC(C)OC(=O)CCC(=O)OC(C#CC)CC</chem>
Mol. weight [g/mol]:	266.33

Physical Properties

Property code	Value	Unit	Source
gf	-106.66	kJ/mol	Joback Method
hf	-455.36	kJ/mol	Joback Method
hfus	34.98	kJ/mol	Joback Method
hvap	68.00	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.619		Crippen Method
mvol	224.190	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	699.98	K	Joback Method
tc	898.37	K	Joback Method
tf	477.47	K	Joback Method
vc	0.855	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.81	J/mol×K	699.98	Joback Method
cpg	625.32	J/mol×K	733.04	Joback Method
cpg	639.96	J/mol×K	766.11	Joback Method
cpg	653.75	J/mol×K	799.17	Joback Method
cpg	666.70	J/mol×K	832.24	Joback Method
cpg	678.82	J/mol×K	865.30	Joback Method
cpg	690.10	J/mol×K	898.37	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=U391156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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