Succinic acid, hex-4-yn-3-yl 3-methylbut-3-en-1-yl ester

Inchi: InChI=1S/C15H22O4/c1-5-7-13(6-2)19-15(17)9-8-14(16)18-11-10-12(3)4/h13H,3,6,8-11H

InchiKey: UOJDEVCATSGCHR-UHFFFAOYSA-N

Formula: C15H22O4

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

Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-112.77	kJ/mol	Joback Method
hf	-459.87	kJ/mol	Joback Method
hfus	37.19	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.621		Crippen Method
mcvol	224.190	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
tb	700.30	K	Joback Method
tc	898.20	K	Joback Method
tf	478.51	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.99	J/mol×K	700.30	Joback Method
cpg	624.41	J/mol×K	733.28	Joback Method
cpg	638.98	J/mol×K	766.27	Joback Method
cpg	652.73	J/mol×K	799.25	Joback Method
cpg	665.65	J/mol×K	832.23	Joback Method
cpg	677.75	J/mol×K	865.21	Joback Method
cpg	689.04	J/mol×K	898.20	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=U391134&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