Succinic acid, but-3-yn-2-yl hept-1,6-dien-4-yl ester

Inchi: InChI=1S/C15H20O4/c1-5-8-13(9-6-2)19-15(17)11-10-14(16)18-12(4)7-3/h3,5-6,12-13H,

InchiKey: NHVZZCZEGOUFQM-UHFFFAOYSA-N

Formula: C15H20O4

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

Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	1.45	kJ/mol	Joback Method
hf	-310.33	kJ/mol	Joback Method
hfus	33.55	kJ/mol	Joback Method
hvap	65.04	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.395		Crippen Method
mcvol	219.890	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	1671.00		NIST Webbook
tb	677.78	K	Joback Method
tc	871.32	K	Joback Method
tf	416.58	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.16	J/mol×K	677.78	Joback Method
cpg	597.70	J/mol×K	710.04	Joback Method
cpg	611.44	J/mol×K	742.29	Joback Method
cpg	624.39	J/mol×K	774.55	Joback Method
cpg	636.58	J/mol×K	806.81	Joback Method
cpg	648.02	J/mol×K	839.06	Joback Method
cpg	658.74	J/mol×K	871.32	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=U391328&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

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