Succinic acid, but-3-yn-2-yl 1-cyclopentylethyl ester

Inchi: InChI=1S/C15H22O4/c1-4-11(2)18-14(16)9-10-15(17)19-12(3)13-7-5-6-8-13/h1,11-13H,5

InchiKey: CLKCQBUQPWBMOH-UHFFFAOYSA-N

Formula: C15H22O4

SMILES: C#CC(C)OC(=O)CCC(=O)OC(C)C1CCCC1

Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-137.68	kJ/mol	Joback Method
hf	-500.71	kJ/mol	Joback Method
hfus	30.04	kJ/mol	Joback Method
hvap	66.64	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.453		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1803.00		NIST Webbook
tb	699.70	K	Joback Method
tc	909.14	K	Joback Method
tf	431.00	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.44	J/mol×K	699.70	Joback Method
cpg	637.71	J/mol×K	734.61	Joback Method
cpg	653.88	J/mol×K	769.51	Joback Method
cpg	668.98	J/mol×K	804.42	Joback Method
cpg	683.03	J/mol×K	839.33	Joback Method
cpg	696.07	J/mol×K	874.23	Joback Method
cpg	708.10	J/mol×K	909.14	Joback Method

Sources

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=U391409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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