

Succinic acid, but-3-yn-2-yl 2-methylpentyl ester

Inchi:	InChI=1S/C14H22O4/c1-5-7-11(3)10-17-13(15)8-9-14(16)18-12(4)6-2/h2,11-12H,5,7-10H
InchiKey:	HRQDMAGRPUUGGK-UHFFFAOYSA-N
Formula:	C14H22O4
SMILES:	C#CC(C)OC(=O)CCC(=O)OCC(C)CCC
Mol. weight [g/mol]:	254.32

Physical Properties

Property code	Value	Unit	Source
gf	-182.65	kJ/mol	Joback Method
hf	-540.55	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.311		Crippen Method
mvol	214.400	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
tb	661.54	K	Joback Method
tc	851.00	K	Joback Method
tf	408.83	K	Joback Method
vc	0.818	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.39	J/molxK	661.54	Joback Method
cpg	591.56	J/molxK	693.12	Joback Method
cpg	605.95	J/molxK	724.69	Joback Method
cpg	619.58	J/molxK	756.27	Joback Method
cpg	632.46	J/molxK	787.85	Joback Method
cpg	644.59	J/molxK	819.43	Joback Method
cpg	655.98	J/molxK	851.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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