Succinic acid, hex-4-yn-3-yl 2-methoxyethyl ester

Inchi: InChI=1S/C13H20O5/c1-4-6-11(5-2)18-13(15)8-7-12(14)17-10-9-16-3/h11H,5,7-10H2,1-3

InchiKey: CSRSYWDFQYIKNQ-UHFFFAOYSA-N

Formula: C13H20O5

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

Mol. weight [g/mol]: 256.29

Physical Properties

Property code	Value	Unit	Source
gf	-313.90	kJ/mol	Joback Method
hf	-666.45	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	67.02	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.301		Crippen Method
mcvol	206.180	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1764.00		NIST Webbook
rinpol	1764.00		NIST Webbook
tb	680.40	K	Joback Method
tc	875.40	K	Joback Method
tf	493.92	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.29	J/mol×K	680.40	Joback Method
cpg	567.88	J/mol×K	712.90	Joback Method
cpg	581.73	J/mol×K	745.40	Joback Method
cpg	594.82	J/mol×K	777.90	Joback Method
cpg	607.14	J/mol×K	810.40	Joback Method
cpg	618.67	J/mol×K	842.90	Joback Method
cpg	629.41	J/mol×K	875.40	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=U390738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume