Succinic acid, but-3-yn-2-yl 4-octyl ester

Inchi: InChI=1S/C16H26O4/c1-5-8-10-14(9-6-2)20-16(18)12-11-15(17)19-13(4)7-3/h3,13-14H,5
InchiKey: KCLZXEWELTXBJS-UHFFFAOYSA-N
Formula: C16H26O4
SMILES: C#CC(C)OC(=O)CCC(=O)OC(CCC)CCCC
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-165.81	kJ/mol	Joback Method
hf	-581.83	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	68.60	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.234		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook
tb	707.30	K	Joback Method
tc	894.24	K	Joback Method
tf	431.37	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.68	J/mol×K	707.30	Joback Method
cpg	700.73	J/mol×K	738.46	Joback Method
cpg	715.93	J/mol×K	769.61	Joback Method
cpg	730.29	J/mol×K	800.77	Joback Method
cpg	743.83	J/mol×K	831.93	Joback Method
cpg	756.57	J/mol×K	863.08	Joback Method
cpg	768.50	J/mol×K	894.24	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=U389555&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