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

Inchi: InChI=1S/C16H26O4/c1-5-8-10-13(4)19-15(17)11-12-16(18)20-14(7-3)9-6-2/h13-14H,5,7
InchiKey: BUTOEINYMOZHSB-UHFFFAOYSA-N
Formula: C16H26O4
SMILES: CC#CC(CC)OC(=O)CCC(=O)OC(C)CCCC
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-186.08	kJ/mol	Joback Method
hf	-601.43	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	70.90	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.234		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	726.18	K	Joback Method
tc	920.20	K	Joback Method
tf	490.50	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.06	J/mol×K	726.18	Joback Method
cpg	705.48	J/mol×K	758.52	Joback Method
cpg	720.99	J/mol×K	790.85	Joback Method
cpg	735.60	J/mol×K	823.19	Joback Method
cpg	749.31	J/mol×K	855.53	Joback Method
cpg	762.13	J/mol×K	887.87	Joback Method
cpg	774.07	J/mol×K	920.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390683&Units=SI
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

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