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

Inchi: InChI=1S/C16H26O4/c1-7-9-13(8-2)20-15(18)11-10-14(17)19-12(3)16(4,5)6/h12-13H,8,1

InchiKey: IHIFITNCJSCRFM-UHFFFAOYSA-N

Formula: C16H26O4

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

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-183.24	kJ/mol	Joback Method
hf	-610.18	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	69.60	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.089		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
tb	722.95	K	Joback Method
tc	925.17	K	Joback Method
tf	492.92	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.25	J/mol×K	722.95	Joback Method
cpg	708.09	J/mol×K	756.65	Joback Method
cpg	723.92	J/mol×K	790.36	Joback Method
cpg	738.77	J/mol×K	824.06	Joback Method
cpg	752.66	J/mol×K	857.76	Joback Method
cpg	765.62	J/mol×K	891.47	Joback Method
cpg	777.66	J/mol×K	925.17	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=U390622&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