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

Inchi: InChI=1S/C18H22O4/c1-5-8-15(6-2)21-17(19)11-12-18(20)22-16-10-7-9-13(3)14(16)4/h7
InchiKey: KVMDHHFRGJDGKJ-UHFFFAOYSA-N
Formula: C18H22O4
SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 302.36

Physical Properties

Property code	Value	Unit	Source
gf	-73.65	kJ/mol	Joback Method
hf	-423.84	kJ/mol	Joback Method
hfus	40.81	kJ/mol	Joback Method
hvap	79.34	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.334		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2247.00		NIST Webbook
rinpol	2247.00		NIST Webbook
tb	809.02	K	Joback Method
tc	1027.64	K	Joback Method
tf	579.50	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.92	J/mol×K	809.02	Joback Method
cpg	726.08	J/mol×K	845.46	Joback Method
cpg	740.10	J/mol×K	881.89	Joback Method
cpg	752.99	J/mol×K	918.33	Joback Method
cpg	764.76	J/mol×K	954.77	Joback Method
cpg	775.41	J/mol×K	991.21	Joback Method
cpg	784.96	J/mol×K	1027.64	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=U390020&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