Succinic acid, tridec-2-yn-1-yl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C25H36O4/c1-4-5-6-7-8-9-10-11-12-13-14-20-28-24(26)18-19-25(27)29-23-17

InchiKey: ZNRVSYYMIAMKIB-UHFFFAOYSA-N

Formula: C25H36O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-12.27	kJ/mol	Joback Method
hf	-563.04	kJ/mol	Joback Method
hfus	62.46	kJ/mol	Joback Method
hvap	95.31	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.066		Crippen Method
mcvol	345.630	ml/mol	McGowan Method
pc	1064.48	kPa	Joback Method
rinpol	3066.00		NIST Webbook
rinpol	3066.00		NIST Webbook
tb	969.62	K	Joback Method
tc	1188.61	K	Joback Method
tf	673.39	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.99	J/mol×K	969.62	Joback Method
cpg	1140.99	J/mol×K	1006.12	Joback Method
cpg	1155.55	J/mol×K	1042.62	Joback Method
cpg	1168.71	J/mol×K	1079.11	Joback Method
cpg	1180.49	J/mol×K	1115.61	Joback Method
cpg	1190.93	J/mol×K	1152.11	Joback Method
cpg	1200.07	J/mol×K	1188.61	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=U390033&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