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

Inchi: InChI=1S/C24H34O5/c1-3-4-5-6-7-8-9-10-11-12-13-19-28-23(25)17-18-24(26)29-22-16-1

InchiKey: WPLMOOSYHNKBHV-UHFFFAOYSA-N

Formula: C24H34O5

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)Oc1cccc(OC)c1

Mol. weight [g/mol]: 402.52

Physical Properties

Property code	Value	Unit	Source
gf	-116.06	kJ/mol	Joback Method
hf	-663.15	kJ/mol	Joback Method
hfus	61.45	kJ/mol	Joback Method
hvap	94.83	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.458		Crippen Method
mcvol	337.410	ml/mol	McGowan Method
pc	1132.91	kPa	Joback Method
rinpol	3086.00		NIST Webbook
rinpol	3086.00		NIST Webbook
tb	964.18	K	Joback Method
tc	1182.27	K	Joback Method
tf	671.83	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.38	J/mol×K	964.18	Joback Method
cpg	1108.57	J/mol×K	1000.53	Joback Method
cpg	1122.26	J/mol×K	1036.88	Joback Method
cpg	1134.46	J/mol×K	1073.23	Joback Method
cpg	1145.20	J/mol×K	1109.57	Joback Method
cpg	1154.50	J/mol×K	1145.92	Joback Method
cpg	1162.38	J/mol×K	1182.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390989&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