

Succinic acid, tridec-2-yn-1-yl 2-methoxy-5-methylphenyl ester

Inchi:	InChI=1S/C25H36O5/c1-4-5-6-7-8-9-10-11-12-13-14-19-29-24(26)17-18-25(27)30-23-20
InchiKey:	GKCXKDKGONFQMI-UHFFFAOYSA-N
Formula:	C25H36O5
SMILES:	CCCCCCCCC#CCOC(=O)CCC(=O)Oc1cc(C)ccc1OC
Mol. weight [g/mol]:	416.55

Physical Properties

Property code	Value	Unit	Source
gf	-117.27	kJ/mol	Joback Method
hf	-695.26	kJ/mol	Joback Method
hfus	63.65	kJ/mol	Joback Method
hvap	97.72	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	5.767		Crippen Method
mcvol	351.500	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	3121.00		NIST Webbook
rinpol	3121.00		NIST Webbook
tb	992.04	K	Joback Method
tc	1214.89	K	Joback Method
tf	695.62	K	Joback Method
vc	1.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.54	J/mol×K	992.04	Joback Method
cpg	1168.65	J/mol×K	1029.18	Joback Method
cpg	1182.13	J/mol×K	1066.32	Joback Method
cpg	1194.01	J/mol×K	1103.47	Joback Method
cpg	1204.29	J/mol×K	1140.61	Joback Method
cpg	1213.00	J/mol×K	1177.75	Joback Method
cpg	1220.15	J/mol×K	1214.89	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=U390970&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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