Succinic acid, hex-4-yn-3-yl 2-methoxy-5-methylphenyl ester

Inchi: InChI=1S/C18H22O5/c1-5-7-14(6-2)22-17(19)10-11-18(20)23-16-12-13(3)8-9-15(16)21-4

InchiKey: LVGKQDCYYIKTMY-UHFFFAOYSA-N

Formula: C18H22O5

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 318.36

Physical Properties

Property code	Value	Unit	Source
gf	-178.65	kJ/mol	Joback Method
hf	-556.06	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	81.75	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.034		Crippen Method
mcvol	252.870	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		NIST Webbook
tb	831.44	K	Joback Method
tc	1048.80	K	Joback Method
tf	601.73	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.57	J/mol×K	831.44	Joback Method
cpg	753.19	J/mol×K	867.67	Joback Method
cpg	766.61	J/mol×K	903.89	Joback Method
cpg	778.82	J/mol×K	940.12	Joback Method
cpg	789.80	J/mol×K	976.35	Joback Method
cpg	799.56	J/mol×K	1012.58	Joback Method
cpg	808.09	J/mol×K	1048.80	Joback Method

Sources

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=U390958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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