Succinic acid, hex-4-yn-3-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H19ClO5/c1-4-6-13(5-2)22-16(19)9-10-17(20)23-14-8-7-12(18)11-15(14)21

InchiKey: RQBDZPDUSMKHGV-UHFFFAOYSA-N

Formula: C17H19ClO5

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 338.78

Physical Properties

Property code	Value	Unit	Source
gf	-199.00	kJ/mol	Joback Method
hf	-551.16	kJ/mol	Joback Method
hfus	43.61	kJ/mol	Joback Method
hvap	83.91	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.379		Crippen Method
mcvol	251.020	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2408.00		NIST Webbook
rinpol	2408.00		NIST Webbook
tb	845.99	K	Joback Method
tc	1068.68	K	Joback Method
tf	620.38	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.33	J/mol×K	845.99	Joback Method
cpg	719.47	J/mol×K	883.11	Joback Method
cpg	731.41	J/mol×K	920.22	Joback Method
cpg	742.15	J/mol×K	957.34	Joback Method
cpg	751.67	J/mol×K	994.45	Joback Method
cpg	759.98	J/mol×K	1031.57	Joback Method
cpg	767.05	J/mol×K	1068.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390936&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