Succinic acid, 3-methylbut-2-en-1-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C16H19ClO5/c1-11(2)8-9-21-15(18)6-7-16(19)22-13-5-4-12(17)10-14(13)20-3/

InchiKey: ICEXRWOTHWBXRQ-UHFFFAOYSA-N

Formula: C16H19ClO5

SMILES: COc1cc(Cl)ccc1OC(=O)CCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 326.77

Physical Properties

Property code	Value	Unit	Source
gf	-336.11	kJ/mol	Joback Method
hf	-690.11	kJ/mol	Joback Method
hfus	40.31	kJ/mol	Joback Method
hvap	79.95	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.544		Crippen Method
mcvol	241.230	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	818.59	K	Joback Method
tc	1032.35	K	Joback Method
tf	498.97	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.77	J/mol×K	818.59	Joback Method
cpg	687.91	J/mol×K	854.22	Joback Method
cpg	700.03	J/mol×K	889.84	Joback Method
cpg	711.13	J/mol×K	925.47	Joback Method
cpg	721.24	J/mol×K	961.10	Joback Method
cpg	730.35	J/mol×K	996.73	Joback Method
cpg	738.47	J/mol×K	1032.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390934&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