Succinic acid, 2,2-dichloroethyl 3-methoxyphenyl ester

Inchi: InChI=1S/C13H14Cl2O5/c1-18-9-3-2-4-10(7-9)20-13(17)6-5-12(16)19-8-11(14)15/h2-4,7

InchiKey: CRGPFGYURXKDME-UHFFFAOYSA-N

Formula: C13H14Cl2O5

SMILES: COc1cccc(OC(=O)CCC(=O)OCC(Cl)Cl)c1

Mol. weight [g/mol]: 321.15

Physical Properties

Property code	Value	Unit	Source
gf	-437.78	kJ/mol	Joback Method
hf	-745.17	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	76.57	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.728		Crippen Method
mcvol	215.500	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook
tb	777.92	K	Joback Method
tc	994.75	K	Joback Method
tf	486.60	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.75	J/mol×K	777.92	Joback Method
cpg	574.44	J/mol×K	814.06	Joback Method
cpg	585.15	J/mol×K	850.20	Joback Method
cpg	594.89	J/mol×K	886.34	Joback Method
cpg	603.64	J/mol×K	922.47	Joback Method
cpg	611.40	J/mol×K	958.61	Joback Method
cpg	618.16	J/mol×K	994.75	Joback Method
dvisc	0.0006326	Pa×s	486.60	Joback Method

dvisc	0.0003784	Pa×s	535.15	Joback Method
dvisc	0.0002466	Pa×s	583.71	Joback Method
dvisc	0.0001716	Pa×s	632.26	Joback Method
dvisc	0.0001257	Pa×s	680.81	Joback Method
dvisc	0.0000960	Pa×s	729.37	Joback Method
dvisc	0.0000759	Pa×s	777.92	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=U390979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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