

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

Inchi:	InChI=1S/C17H14Cl2O5/c1-22-12-6-2-3-7-13(12)23-15(20)9-10-16(21)24-14-8-4-5-11(18)
InchiKey:	DZUMVDLRRQNNOD-UHFFFAOYSA-N
Formula:	C17H14Cl2O5
SMILES:	COc1ccccc1OC(=O)CCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	369.20

Physical Properties

Property code	Value	Unit	Source
gf	-308.51	kJ/mol	Joback Method
hf	-608.86	kJ/mol	Joback Method
hfus	41.86	kJ/mol	Joback Method
hvap	89.47	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.293		Crippen Method
mvol	248.100	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	2814.00		NIST Webbook
rinpol	2814.00		NIST Webbook
tb	906.52	K	Joback Method
tc	1143.16	K	Joback Method
tf	598.14	K	Joback Method
vc	0.935	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.45	J/molxK	906.52	Joback Method
cpg	715.84	J/molxK	1103.72	Joback Method
cpg	711.00	J/molxK	1064.28	Joback Method
cpg	704.84	J/molxK	1024.84	Joback Method
cpg	697.36	J/molxK	985.40	Joback Method
cpg	688.56	J/molxK	945.96	Joback Method
cpg	719.36	J/molxK	1143.16	Joback Method
dvisc	0.0000497	Paxs	906.52	Joback Method

dvisc	0.0000607	Paxs	855.12	Joback Method
dvisc	0.0000761	Paxs	803.73	Joback Method
dvisc	0.0000984	Paxs	752.33	Joback Method
dvisc	0.0001322	Paxs	700.93	Joback Method
dvisc	0.0001860	Paxs	649.54	Joback Method
dvisc	0.0002776	Paxs	598.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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

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