

Succinic acid, 2,3-dichlorophenyl non-3-en-1-yl ester

Inchi:	InChI=1S/C19H24Cl2O4/c1-2-3-4-5-6-7-8-14-24-17(22)12-13-18(23)25-16-11-9-10-15(20)
InchiKey:	ZTJAFNKVTQDHDU-VOTSOKGWSA-N
Formula:	C19H24Cl2O4
SMILES:	CCCCC=CCCOC(=O)CCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	387.30

Physical Properties

Property code	Value	Unit	Source
gf	-209.23	kJ/mol	Joback Method
hf	-625.76	kJ/mol	Joback Method
hfus	52.40	kJ/mol	Joback Method
hvap	88.53	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.749		Crippen Method
mcvol	289.870	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2755.00		NIST Webbook
rinpol	2755.00		NIST Webbook
tb	902.36	K	Joback Method
tc	1116.64	K	Joback Method
tf	554.43	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.57	J/molxK	902.36	Joback Method
cpg	897.99	J/molxK	1080.93	Joback Method
cpg	888.86	J/molxK	1045.21	Joback Method
cpg	878.79	J/molxK	1009.50	Joback Method
cpg	867.74	J/molxK	973.79	Joback Method
cpg	855.68	J/molxK	938.07	Joback Method
cpg	906.21	J/molxK	1116.64	Joback Method
dvisc	0.0000416	Paxs	902.36	Joback Method

dvisc	0.0000526	Paxs	844.37	Joback Method
dvisc	0.0000688	Paxs	786.38	Joback Method
dvisc	0.0000941	Paxs	728.39	Joback Method
dvisc	0.0001357	Paxs	670.41	Joback Method
dvisc	0.0002099	Paxs	612.42	Joback Method
dvisc	0.0003555	Paxs	554.43	Joback Method

Sources

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=U391101&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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