

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

Inchi:	InChI=1S/C19H18Cl2O5/c1-12(2)24-14-7-3-4-8-15(14)25-17(22)10-11-18(23)26-16-9-5-6
InchiKey:	BKPMGRZDLGJHDL-UHFFFAOYSA-N
Formula:	C19H18Cl2O5
SMILES:	CC(C)Oc1ccccc1OC(=O)CCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	397.25

Physical Properties

Property code	Value	Unit	Source
gf	-294.11	kJ/mol	Joback Method
hf	-655.42	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	93.53	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.072		Crippen Method
mcvol	276.280	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	2870.00		NIST Webbook
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tb	951.84	K	Joback Method
tc	1187.60	K	Joback Method
tf	605.68	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.56	J/molxK	951.84	Joback Method
cpg	801.88	J/molxK	991.13	Joback Method
cpg	810.74	J/molxK	1030.43	Joback Method
cpg	818.18	J/molxK	1069.72	Joback Method
cpg	824.20	J/molxK	1109.02	Joback Method
cpg	828.80	J/molxK	1148.31	Joback Method
cpg	832.00	J/molxK	1187.60	Joback Method
dvisc	0.0002393	Paxs	605.68	Joback Method

dvisc	0.0001500	Paxs	663.37	Joback Method
dvisc	0.0001014	Paxs	721.07	Joback Method
dvisc	0.0000726	Paxs	778.76	Joback Method
dvisc	0.0000544	Paxs	836.45	Joback Method
dvisc	0.0000423	Paxs	894.15	Joback Method
dvisc	0.0000340	Paxs	951.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357975&Units=SI

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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