

Succinic acid, 2,3-dichlorophenyl 4-isopropylphenyl ester

Inchi:	InChI=1S/C19H18Cl2O4/c1-12(2)13-6-8-14(9-7-13)24-17(22)10-11-18(23)25-16-5-3-4-15
InchiKey:	VHAPDIVSIRCYSZ-UHFFFAOYSA-N
Formula:	C19H18Cl2O4
SMILES:	CC(C)c1ccc(OC(=O)CCC(=O)Oc2cccc(Cl)c2Cl)cc1
Mol. weight [g/mol]:	381.25

Physical Properties

Property code	Value	Unit	Source
gf	-189.11	kJ/mol	Joback Method
hf	-523.20	kJ/mol	Joback Method
hfus	42.33	kJ/mol	Joback Method
hvap	91.12	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.408		Crippen Method
mcvol	270.410	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinqol	2867.00		NIST Webbook
tb	929.42	K	Joback Method
tc	1166.09	K	Joback Method
tf	583.45	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.38	J/molxK	929.42	Joback Method
cpg	777.59	J/molxK	968.87	Joback Method
cpg	787.48	J/molxK	1008.31	Joback Method
cpg	796.10	J/molxK	1047.76	Joback Method
cpg	803.46	J/molxK	1087.20	Joback Method
cpg	809.61	J/molxK	1126.65	Joback Method
cpg	814.58	J/molxK	1166.09	Joback Method
dvisc	0.0003363	Paxs	583.45	Joback Method
dvisc	0.0002076	Paxs	641.11	Joback Method

dvisc	0.0001387	Paxs	698.77	Joback Method
dvisc	0.0000986	Paxs	756.44	Joback Method
dvisc	0.0000736	Paxs	814.10	Joback Method
dvisc	0.0000570	Paxs	871.76	Joback Method
dvisc	0.0000457	Paxs	929.42	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=U360722&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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