Succinic acid, phenyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C16H12Cl2O4/c17-12-7-4-8-13(16(12)18)22-15(20)10-9-14(19)21-11-5-2-1-3-6
InchiKey: WGOJWQPZCRSLDC-UHFFFAOYSA-N
Formula: C16H12Cl2O4
SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)Oc1ccccc1
Mol. weight [g/mol]: 339.17

Physical Properties

Property code	Value	Unit	Source
gf	-202.30	kJ/mol	Joback Method
hf	-444.53	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	84.17	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.285		Crippen Method
mcvol	228.140	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook
tb	856.24	K	Joback Method
tc	1097.45	K	Joback Method
tf	552.12	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.36	J/mol×K	856.24	Joback Method
cpg	611.06	J/mol×K	896.44	Joback Method
cpg	620.57	J/mol×K	936.64	Joback Method
cpg	628.93	J/mol×K	976.84	Joback Method
cpg	636.16	J/mol×K	1017.04	Joback Method
cpg	642.29	J/mol×K	1057.25	Joback Method
cpg	647.35	J/mol×K	1097.45	Joback Method
dvisc	0.0004711	Pa×s	552.12	Joback Method

dvisc	0.0003047	Pa×s	602.81	Joback Method
dvisc	0.0002109	Pa×s	653.49	Joback Method
dvisc	0.0001539	Pa×s	704.18	Joback Method
dvisc	0.0001172	Pa×s	754.87	Joback Method
dvisc	0.0000923	Pa×s	805.55	Joback Method
dvisc	0.0000748	Pa×s	856.24	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=U357994&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

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