

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
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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/molxK	856.24	Joback Method
cpg	642.29	J/molxK	1057.25	Joback Method
cpg	636.16	J/molxK	1017.04	Joback Method
cpg	628.93	J/molxK	976.84	Joback Method
cpg	620.57	J/molxK	936.64	Joback Method
cpg	611.06	J/molxK	896.44	Joback Method
cpg	647.35	J/molxK	1097.45	Joback Method
dvisc	0.0000748	Paxs	856.24	Joback Method

dvisc	0.0000923	Paxs	805.55	Joback Method
dvisc	0.0001172	Paxs	754.87	Joback Method
dvisc	0.0001539	Paxs	704.18	Joback Method
dvisc	0.0002109	Paxs	653.49	Joback Method
dvisc	0.0003047	Paxs	602.81	Joback Method
dvisc	0.0004711	Paxs	552.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357994&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

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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