

Succinic acid, 3-chlorophenyl 3,5-dichlorophenyl ester

Inchi: InChI=1S/C16H11Cl3O4/c17-10-2-1-3-13(7-10)22-15(20)4-5-16(21)23-14-8-11(18)6-12(19)
InchiKey: OKIKEGRNHRAVRT-UHFFFAOYSA-N
Formula: C16H11Cl3O4
SMILES: O=C(CCC(=O)Oc1cc(Cl)cc(Cl)c1)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 373.62

Physical Properties

Property code	Value	Unit	Source
gf	-223.86	kJ/mol	Joback Method
hf	-471.74	kJ/mol	Joback Method
hfus	42.28	kJ/mol	Joback Method
hvap	89.21	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.938		Crippen Method
mcvol	240.380	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	2680.00		NIST Webbook
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tb	898.65	K	Joback Method
tc	1142.90	K	Joback Method
tf	594.56	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.57	J/molxK	898.65	Joback Method
cpg	626.83	J/molxK	939.36	Joback Method
cpg	634.92	J/molxK	980.07	Joback Method
cpg	641.86	J/molxK	1020.78	Joback Method
cpg	647.66	J/molxK	1061.49	Joback Method
cpg	652.35	J/molxK	1102.20	Joback Method
cpg	655.95	J/molxK	1142.90	Joback Method
dvisc	0.0003592	Paxs	594.56	Joback Method

dvisc	0.0002423	Paxs	645.24	Joback Method
dvisc	0.0001731	Paxs	695.92	Joback Method
dvisc	0.0001294	Paxs	746.61	Joback Method
dvisc	0.0001004	Paxs	797.29	Joback Method
dvisc	0.0000803	Paxs	847.97	Joback Method
dvisc	0.0000659	Paxs	898.65	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=U390155&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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