

Succinic acid, 8-chlorooctyl 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C18H22Cl4O4/c19-9-5-3-1-2-4-6-10-25-17(23)7-8-18(24)26-16-12-14(21)13(20)
InchiKey:	GZCDARYEONVSMK-UHFFFAOYSA-N
Formula:	C18H22Cl4O4
SMILES:	O=C(CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)OCCCCCCCCCl
Mol. weight [g/mol]:	444.18

Physical Properties

Property code	Value	Unit	Source
gf	-331.36	kJ/mol	Joback Method
hf	-765.29	kJ/mol	Joback Method
hfus	57.61	kJ/mol	Joback Method
hvap	95.78	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.455		Crippen Method
mvol	304.560	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	3031.00		NIST Webbook
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tb	955.16	K	Joback Method
tc	1176.10	K	Joback Method
tf	620.60	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.38	J/molxK	955.16	Joback Method
cpg	898.35	J/molxK	1139.28	Joback Method
cpg	891.97	J/molxK	1102.45	Joback Method
cpg	884.51	J/molxK	1065.63	Joback Method
cpg	875.93	J/molxK	1028.81	Joback Method
cpg	866.23	J/molxK	991.98	Joback Method
cpg	903.65	J/molxK	1176.10	Joback Method
dvisc	0.0000404	Paxs	955.16	Joback Method

dvisc	0.0000500	Paxs	899.40	Joback Method
dvisc	0.0000638	Paxs	843.64	Joback Method
dvisc	0.0000842	Paxs	787.88	Joback Method
dvisc	0.0001159	Paxs	732.12	Joback Method
dvisc	0.0001682	Paxs	676.36	Joback Method
dvisc	0.0002609	Paxs	620.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389975&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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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