

Succinic acid, ethyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C12H11Cl3O4/c1-2-18-10(16)3-4-11(17)19-9-6-7(13)5-8(14)12(9)15/h5-6H,2-4
InchiKey: DMGJAPZJPKIMQE-UHFFFAOYSA-N
Formula: C12H11Cl3O4
SMILES: CCOC(=O)CCC(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 325.57

Physical Properties

Property code	Value	Unit	Source
gf	-369.95	kJ/mol	Joback Method
hf	-625.71	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	78.03	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.896		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	2116.00		NIST Webbook
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tb	780.45	K	Joback Method
tc	1003.15	K	Joback Method
tf	523.06	K	Joback Method
vc	0.794	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.14	J/molxK	780.45	Joback Method
cpg	545.24	J/molxK	966.04	Joback Method
cpg	538.53	J/molxK	928.92	Joback Method
cpg	530.96	J/molxK	891.80	Joback Method
cpg	522.53	J/molxK	854.68	Joback Method
cpg	513.26	J/molxK	817.57	Joback Method
cpg	551.09	J/molxK	1003.15	Joback Method
dvisc	0.0001107	Paxs	780.45	Joback Method

dvisc	0.0001341	Paxs	737.55	Joback Method
dvisc	0.0001663	Paxs	694.65	Joback Method
dvisc	0.0002121	Paxs	651.75	Joback Method
dvisc	0.0002801	Paxs	608.86	Joback Method
dvisc	0.0003857	Paxs	565.96	Joback Method
dvisc	0.0005598	Paxs	523.06	Joback Method

Sources

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=U349605&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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