

Succinic acid, 3-chlorophenyl 10-chlorodecyl ester

Inchi:	InChI=1S/C20H28Cl2O4/c21-14-7-5-3-1-2-4-6-8-15-25-19(23)12-13-20(24)26-18-11-9-10
InchiKey:	SRPLGDCKHQLAFE-UHFFFAOYSA-N
Formula:	C20H28Cl2O4
SMILES:	O=C(CCC(=O)Oc1cccc(Cl)c1)OCCCCCCCCCCI
Mol. weight [g/mol]:	403.34

Physical Properties

Property code	Value	Unit	Source
gf	-271.40	kJ/mol	Joback Method
hf	-752.15	kJ/mol	Joback Method
hfus	55.18	kJ/mol	Joback Method
hvap	90.13	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.928		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	2996.00		NIST Webbook
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tb	916.10	K	Joback Method
tc	1127.16	K	Joback Method
tf	558.26	K	Joback Method
vc	1.194	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.17	J/molxK	916.10	Joback Method
cpg	987.77	J/molxK	1091.99	Joback Method
cpg	978.47	J/molxK	1056.81	Joback Method
cpg	968.09	J/molxK	1021.63	Joback Method
cpg	956.60	J/molxK	986.45	Joback Method
cpg	943.97	J/molxK	951.28	Joback Method
cpg	996.01	J/molxK	1127.16	Joback Method
dvisc	0.0000402	Paxs	916.10	Joback Method

dvisc	0.0000515	Paxs	856.46	Joback Method
dvisc	0.0000685	Paxs	796.82	Joback Method
dvisc	0.0000953	Paxs	737.18	Joback Method
dvisc	0.0001405	Paxs	677.54	Joback Method
dvisc	0.0002234	Paxs	617.90	Joback Method
dvisc	0.0003923	Paxs	558.26	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=U390415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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