

Succinic acid, 3-chlorophenyl 4-biphenyl ester

Inchi: InChI=1S/C22H17ClO4/c23-18-7-4-8-20(15-18)27-22(25)14-13-21(24)26-19-11-9-17(10-13)/1-2
InchiKey: NROIRGOBMMQAFT-UHFFFAOYSA-N
Formula: C22H17ClO4
SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 380.82

Physical Properties

Property code	Value	Unit	Source
gf	-27.44	kJ/mol	Joback Method
hf	-316.10	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	95.41	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.298		Crippen Method
mvol	276.680	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	3303.00		NIST Webbook
rinpol	3303.00		NIST Webbook
tb	982.77	K	Joback Method
tc	1235.65	K	Joback Method
tf	616.24	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.53	J/molxK	982.77	Joback Method
cpg	821.99	J/molxK	1024.92	Joback Method
cpg	831.01	J/molxK	1067.06	Joback Method
cpg	838.65	J/molxK	1109.21	Joback Method
cpg	845.00	J/molxK	1151.36	Joback Method
cpg	850.12	J/molxK	1193.51	Joback Method
cpg	854.09	J/molxK	1235.65	Joback Method
dvisc	0.0002817	Paxs	616.24	Joback Method

dvisc	0.0001741	Paxs	677.33	Joback Method
dvisc	0.0001165	Paxs	738.42	Joback Method
dvisc	0.0000829	Paxs	799.50	Joback Method
dvisc	0.0000619	Paxs	860.59	Joback Method
dvisc	0.0000481	Paxs	921.68	Joback Method
dvisc	0.0000385	Paxs	982.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390090&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
mccvol:	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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