

Succinic acid, di(3-chlorophenethyl) ester

Inchi: InChI=1S/C20H20Cl2O4/c21-17-5-1-3-15(13-17)9-11-25-19(23)7-8-20(24)26-12-10-16-4
InchiKey: SPSPXJOGMONXQB-UHFFFAOYSA-N
Formula: C20H20Cl2O4
SMILES: O=C(CCC(=O)OCCc1cccc(Cl)c1)OCCc1cccc(Cl)c1
Mol. weight [g/mol]: 395.28

Physical Properties

Property code	Value	Unit	Source
gf	-168.62	kJ/mol	Joback Method
hf	-527.09	kJ/mol	Joback Method
hfus	48.83	kJ/mol	Joback Method
hvap	93.07	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.645		Crippen Method
mvol	284.500	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	2975.00		NIST Webbook
rinpol	2975.00		NIST Webbook
tb	947.76	K	Joback Method
tc	1179.66	K	Joback Method
tf	597.20	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.58	J/molxK	947.76	Joback Method
cpg	835.91	J/molxK	986.41	Joback Method
cpg	845.98	J/molxK	1025.06	Joback Method
cpg	854.83	J/molxK	1063.71	Joback Method
cpg	862.49	J/molxK	1102.36	Joback Method
cpg	869.01	J/molxK	1141.01	Joback Method
cpg	874.43	J/molxK	1179.66	Joback Method
dvisc	0.0003147	Paxs	597.20	Joback Method

dvisc	0.0001941	Paxs	655.63	Joback Method
dvisc	0.0001296	Paxs	714.05	Joback Method
dvisc	0.0000920	Paxs	772.48	Joback Method
dvisc	0.0000685	Paxs	830.91	Joback Method
dvisc	0.0000530	Paxs	889.33	Joback Method
dvisc	0.0000424	Paxs	947.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381510&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

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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