

Succinic acid, 3-chlorophenyl tetrahydrofurfuryl ester

Inchi:	InChI=1S/C15H17ClO5/c16-11-3-1-4-12(9-11)21-15(18)7-6-14(17)20-10-13-5-2-8-19-13
InchiKey:	WPGQWRPZWJOQNS-UHFFFAOYSA-N
Formula:	C15H17ClO5
SMILES:	O=C(CCC(=O)Oc1cccc(Cl)c1)OCC1CCCO1
Mol. weight [g/mol]:	312.75

Physical Properties

Property code	Value	Unit	Source
gf	-351.14	kJ/mol	Joback Method
hf	-704.73	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	79.39	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.748		Crippen Method
mvol	220.580	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
tb	806.50	K	Joback Method
tc	1034.20	K	Joback Method
tf	509.46	K	Joback Method
vc	0.827	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.61	J/molxK	806.50	Joback Method
cpg	696.92	J/molxK	996.25	Joback Method
cpg	687.82	J/molxK	958.30	Joback Method
cpg	677.56	J/molxK	920.35	Joback Method
cpg	666.13	J/molxK	882.40	Joback Method
cpg	653.49	J/molxK	844.45	Joback Method
cpg	704.89	J/molxK	1034.20	Joback Method
dvisc	0.0001223	Paxs	806.50	Joback Method

dvisc	0.0001529	Paxs	756.99	Joback Method
dvisc	0.0001971	Paxs	707.49	Joback Method
dvisc	0.0002641	Paxs	657.98	Joback Method
dvisc	0.0003711	Paxs	608.47	Joback Method
dvisc	0.0005538	Paxs	558.97	Joback Method
dvisc	0.0008934	Paxs	509.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390722&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
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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