

Succinic acid, 2-chloro-5-methylphenyl ethyl ester

Inchi:	InChI=1S/C13H15ClO4/c1-3-17-12(15)6-7-13(16)18-11-8-9(2)4-5-10(11)14/h4-5,8H,3,6-
InchiKey:	GHDIOAUFCRONLN-UHFFFAOYSA-N
Formula:	C13H15ClO4
SMILES:	CCOC(=O)CCC(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	270.71

Physical Properties

Property code	Value	Unit	Source
gf	-328.04	kJ/mol	Joback Method
hf	-603.40	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.897		Crippen Method
mcvol	197.390	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	1909.00		NIST Webbook
tb	723.49	K	Joback Method
tc	936.31	K	Joback Method
tf	461.97	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.87	J/mol×K	723.49	Joback Method
cpg	524.64	J/mol×K	758.96	Joback Method
cpg	536.55	J/mol×K	794.43	Joback Method
cpg	547.60	J/mol×K	829.90	Joback Method
cpg	557.80	J/mol×K	865.37	Joback Method
cpg	567.14	J/mol×K	900.84	Joback Method
cpg	575.62	J/mol×K	936.31	Joback Method
dvisc	0.0007813	Pa×s	461.97	Joback Method
dvisc	0.0005017	Pa×s	505.56	Joback Method

dvisc	0.0003456	Pa×s	549.14	Joback Method
dvisc	0.0002515	Pa×s	592.73	Joback Method
dvisc	0.0001912	Pa×s	636.32	Joback Method
dvisc	0.0001505	Pa×s	679.90	Joback Method
dvisc	0.0001220	Pa×s	723.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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