Succinic acid, 3-chlorobenzyl ethyl ester

Inchi: InChI=1S/C13H15ClO4/c1-2-17-12(15)6-7-13(16)18-9-10-4-3-5-11(14)8-10/h3-5,8H,2,6-
InchiKey: CLWGWBXPCUWFGP-UHFFFAOYSA-N
Formula: C13H15ClO4
SMILES: CCOC(=O)CCC(=O)OCc1cccc(Cl)c1
Mol. weight [g/mol]: 270.71

Physical Properties

Property code	Value	Unit	Source
gf	-318.41	kJ/mol	Joback Method
hf	-591.93	kJ/mol	Joback Method
hfus	32.85	kJ/mol	Joback Method
hvap	70.17	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.726		Crippen Method
mcvol	197.390	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	718.51	K	Joback Method
tc	930.52	K	Joback Method
tf	449.45	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.07	J/mol×K	718.51	Joback Method
cpg	568.79	J/mol×K	895.19	Joback Method
cpg	559.38	J/mol×K	859.85	Joback Method
cpg	549.10	J/mol×K	824.52	Joback Method
cpg	537.96	J/mol×K	789.18	Joback Method
cpg	525.96	J/mol×K	753.85	Joback Method
cpg	577.36	J/mol×K	930.52	Joback Method
dvisc	0.0001220	Pa×s	718.51	Joback Method

dvisc	0.0001527	Pa×s	673.67	Joback Method
dvisc	0.0001974	Pa×s	628.82	Joback Method
dvisc	0.0002654	Pa×s	583.98	Joback Method
dvisc	0.0003749	Pa×s	539.14	Joback Method
dvisc	0.0005638	Pa×s	494.29	Joback Method
dvisc	0.0009197	Pa×s	449.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381697&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