Succinic acid, 3-chlorophenyl cyclopentyl ester

Inchi: InChI=1S/C15H17ClO4/c16-11-4-3-7-13(10-11)20-15(18)9-8-14(17)19-12-5-1-2-6-12/h3-

InchiKey: XWLBYZDZZKSFIW-UHFFFAOYSA-N

Formula: C15H17ClO4

SMILES: O=C(CCC(=O)OC1CCCC1)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-265.02	kJ/mol	Joback Method
hf	-572.73	kJ/mol	Joback Method
hfus	31.96	kJ/mol	Joback Method
hvap	74.88	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.511		Crippen Method
mcvol	214.710	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
tb	779.55	K	Joback Method
tc	1009.41	K	Joback Method
tf	482.89	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.69	J/mol×K	779.55	Joback Method
cpg	624.49	J/mol×K	817.86	Joback Method
cpg	638.04	J/mol×K	856.17	Joback Method
cpg	650.37	J/mol×K	894.48	Joback Method
cpg	661.50	J/mol×K	932.79	Joback Method
cpg	671.46	J/mol×K	971.10	Joback Method
cpg	680.30	J/mol×K	1009.41	Joback Method
dvisc	0.0010162	Pa×s	482.89	Joback Method

dvisc	0.0006254	Pa×s	532.33	Joback Method
dvisc	0.0004180	Pa×s	581.78	Joback Method
dvisc	0.0002976	Pa×s	631.22	Joback Method
dvisc	0.0002226	Pa×s	680.66	Joback Method
dvisc	0.0001731	Pa×s	730.11	Joback Method
dvisc	0.0001391	Pa×s	779.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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