Di-(2-o-chlorophenyl-ethylene)-ketone

Inchi: InChI=1S/C17H12Cl2O/c18-16-7-3-1-5-13(16)9-11-15(20)12-10-14-6-2-4-8-17(14)19/h1-
InchiKey: OZBIBYIDJNVAOQ-WGDLNXRISA-N
Formula: C17H12Cl2O
SMILES: O=C(C=Cc1ccccc1Cl)C=Cc1ccccc1Cl
Mol. weight [g/mol]: 303.18
CAS: 5332-98-9

Physical Properties

Property code	Value	Unit	Source
gf	305.48	kJ/mol	Joback Method
hf	146.29	kJ/mol	Joback Method
hfus	37.49	kJ/mol	Joback Method
hvap	74.74	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.289		Crippen Method
mcvol	220.320	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
tb	788.73	K	Joback Method
tc	1045.01	K	Joback Method
tf	458.84	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.01	J/mol×K	788.73	Joback Method
cpg	555.80	J/mol×K	831.44	Joback Method
cpg	567.58	J/mol×K	874.16	Joback Method
cpg	578.47	J/mol×K	916.87	Joback Method
cpg	588.61	J/mol×K	959.59	Joback Method
cpg	598.14	J/mol×K	1002.30	Joback Method
cpg	607.20	J/mol×K	1045.01	Joback Method
dvisc	0.0007971	Pa×s	458.84	Joback Method
dvisc	0.0004537	Pa×s	513.82	Joback Method

dvisc	0.0002879	Pa×s	568.80	Joback Method
dvisc	0.0001980	Pa×s	623.79	Joback Method
dvisc	0.0001447	Pa×s	678.77	Joback Method
dvisc	0.0001108	Pa×s	733.75	Joback Method
dvisc	0.0000881	Pa×s	788.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5332989&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume