Phenyl-(2,4-dichlorophenyl)carbinol

Inchi: InChI=1S/C13H10Cl2O/c14-10-6-7-11(12(15)8-10)13(16)9-4-2-1-3-5-9/h1-8,13,16H
InchiKey: KOMWHXYBCOVOGL-UHFFFAOYSA-N
Formula: C13H10Cl2O
SMILES: OC(c1ccccc1)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 253.12

Physical Properties

Property code	Value	Unit	Source
gf	101.02	kJ/mol	Joback Method
hf	-50.52	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.075		Crippen Method
mcvol	176.860	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	2402.00		NIST Webbook
ripol	3325.00		NIST Webbook
tb	726.76	K	Joback Method
tc	962.34	K	Joback Method
tf	419.81	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.90	J/mol×K	726.76	Joback Method
cpg	469.29	J/mol×K	923.07	Joback Method
cpg	461.56	J/mol×K	883.81	Joback Method
cpg	453.12	J/mol×K	844.55	Joback Method
cpg	443.90	J/mol×K	805.29	Joback Method
cpg	433.85	J/mol×K	766.02	Joback Method
cpg	476.38	J/mol×K	962.34	Joback Method
dvisc	0.0000378	Pa×s	726.76	Joback Method

dvisc	0.0000551	Pa×s	675.60	Joback Method
dvisc	0.0000852	Pa×s	624.44	Joback Method
dvisc	0.0001425	Pa×s	573.29	Joback Method
dvisc	0.0002635	Pa×s	522.13	Joback Method
dvisc	0.0005572	Pa×s	470.97	Joback Method
dvisc	0.0014138	Pa×s	419.81	Joback Method

Sources

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=R537781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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