Dichlorophen, O-(cyclohexanecarbonyl)-

Inchi: InChI=1S/C20H20Cl2O3/c21-16-6-8-18(23)14(11-16)10-15-12-17(22)7-9-19(15)25-20(24
InchiKey: XSNXZTZPLIYJMO-UHFFFAOYSA-N
Formula: C20H20Cl2O3
SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1O)C1CCCCC1
Mol. weight [g/mol]: 379.28

Physical Properties

Property code	Value	Unit	Source
gf	-74.50	kJ/mol	Joback Method
hf	-416.75	kJ/mol	Joback Method
hfus	43.27	kJ/mol	Joback Method
hvap	98.02	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.776		Crippen Method
mcvol	272.070	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook
tb	976.62	K	Joback Method
tc	1237.72	K	Joback Method
tf	656.66	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.93	J/mol×K	976.62	Joback Method
cpg	842.84	J/mol×K	1020.14	Joback Method
cpg	855.78	J/mol×K	1063.65	Joback Method
cpg	867.90	J/mol×K	1107.17	Joback Method
cpg	879.34	J/mol×K	1150.68	Joback Method
cpg	890.26	J/mol×K	1194.20	Joback Method
cpg	900.81	J/mol×K	1237.72	Joback Method
dvisc	0.0000332	Pa×s	656.66	Joback Method

dvisc	0.0000178	Pa×s	709.99	Joback Method
dvisc	0.0000104	Pa×s	763.31	Joback Method
dvisc	0.0000065	Pa×s	816.64	Joback Method
dvisc	0.0000043	Pa×s	869.97	Joback Method
dvisc	0.0000030	Pa×s	923.29	Joback Method
dvisc	0.0000022	Pa×s	976.62	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=U354656&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