Diniconazole

Other names: (E)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-1-yl)-1-penten-3-ol
Inchi: InChI=1S/C15H17Cl2N3O/c1-15(2,3)14(21)13(20-9-18-8-19-20)6-10-4-5-11(16)7-12(10)
InchiKey: FBOUIAKEJMZPQG-AWNIVKPZSA-N
Formula: C15H17Cl2N3O
SMILES: CC(C)(C)C(O)C(=Cc1ccc(Cl)cc1Cl)n1cncn1
Mol. weight [g/mol]: 326.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.66		Crippen Method
logp	3.990		Crippen Method
mcvol	234.980	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	360.40	J/mol×K	283.15	Thermodynamic properties of diniconazole and hexaconazole
cps	367.41	J/mol×K	288.15	Thermodynamic properties of diniconazole and hexaconazole
cps	374.58	J/mol×K	293.15	Thermodynamic properties of diniconazole and hexaconazole
cps	381.72	J/mol×K	298.15	Thermodynamic properties of diniconazole and hexaconazole
cps	388.72	J/mol×K	303.15	Thermodynamic properties of diniconazole and hexaconazole
cps	395.47	J/mol×K	308.15	Thermodynamic properties of diniconazole and hexaconazole

cps	401.89	J/mol×K	313.15	Thermodynamic properties of diniconazole and hexaconazole
cps	407.93	J/mol×K	318.15	Thermodynamic properties of diniconazole and hexaconazole
cps	413.60	J/mol×K	323.15	Thermodynamic properties of diniconazole and hexaconazole
cps	418.90	J/mol×K	328.15	Thermodynamic properties of diniconazole and hexaconazole
cps	423.89	J/mol×K	333.15	Thermodynamic properties of diniconazole and hexaconazole
cps	428.65	J/mol×K	338.15	Thermodynamic properties of diniconazole and hexaconazole
cps	433.27	J/mol×K	343.15	Thermodynamic properties of diniconazole and hexaconazole
cps	437.91	J/mol×K	348.15	Thermodynamic properties of diniconazole and hexaconazole
cps	442.73	J/mol×K	353.15	Thermodynamic properties of diniconazole and hexaconazole
rhos	1323.00	kg/m3	296.00	Thermodynamic properties of diniconazole and hexaconazole

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of diniconazole and hexaconazole:	https://www.doi.org/10.1016/j.jct.2016.04.001
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cps:	Solid phase heat capacity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhos:	Solid Density