2,5-Dianilino-3,6-dichloro hydroquinone

Inchi: InChI=1S/C18H14Cl2N2O2/c19-13-15(21-11-7-3-1-4-8-11)17(23)14(20)16(18(13)24)22-
InchiKey: GKSAMJFHCPTQOS-UHFFFAOYSA-N
Formula: C18H14Cl2N2O2
SMILES: Oc1c(Cl)c(Nc2ccccc2)c(O)c(Cl)c1Nc1ccccc1
Mol. weight [g/mol]: 361.22
CAS: 101716-14-7

Physical Properties

Property code	Value	Unit	Source
gf	254.70	kJ/mol	Joback Method
hf	-18.83	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	112.15	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.892		Crippen Method
mcvol	249.380	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	1042.66	K	Joback Method
tc	1316.80	K	Joback Method
tf	798.04	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.61	J/mol×K	1042.66	Joback Method
cpg	746.12	J/mol×K	1088.35	Joback Method
cpg	761.32	J/mol×K	1134.04	Joback Method
cpg	777.51	J/mol×K	1179.73	Joback Method
cpg	794.98	J/mol×K	1225.42	Joback Method
cpg	814.02	J/mol×K	1271.11	Joback Method
cpg	834.93	J/mol×K	1316.80	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=C101716147&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
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