Clofedanol

Other names:	Benzenemethanol, 2-chloro-«alpha»-[2-(dimethylamino)ethyl]-«alpha»-phenyl- «alpha»-(Dimethylaminoethyl)-o-chlorobenzhydrol Benzhydrol, 2-chloro-«alpha»-(2-(dimethylamino)ethyl)- Chlofedanol Chlophedianol Clophedianol base Dencyl SL 501 base Tussistop Ulo base 2-Chloro-«alpha»-(2-dimethylaminoethyl)benzhydrol Calmotusin Clofedianolo 2-Cloro-«alpha»-(2-dimetilaminoetil)-benzidrolo 1-Phenyl-1-(o-chlorophenyl)-3-dimethylaminopropanol NSC 113595 clofedano
Inchi:	InChI=1S/C17H20ClNO/c1-19(2)13-12-17(20,14-8-4-3-5-9-14)15-10-6-7-11-16(15)18/h3-
InchiKey:	WRCHFMBCVFFYEQ-UHFFFAOYSA-N
Formula:	C17H20ClNO
SMILES:	CN(C)CCC(O)(c1ccccc1)c1ccccc1Cl
Mol. weight [g/mol]:	289.80
CAS:	791-35-5

Physical Properties

Property code	Value	Unit	Source
gf	272.32	kJ/mol	Joback Method
hf	-41.81	kJ/mol	Joback Method
hfus	31.37	kJ/mol	Joback Method
hvap	80.46	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.528		Crippen Method
mcvol	230.960	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook
rinpol	2080.00		NIST Webbook

rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2070.00		NIST Webbook
tb	785.52	K	Joback Method
tc	1006.95	K	Joback Method
tf	472.34	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.52	J/mol×K	785.52	Joback Method
cpg	667.59	J/mol×K	822.43	Joback Method
cpg	680.64	J/mol×K	859.33	Joback Method
cpg	692.75	J/mol×K	896.24	Joback Method
cpg	704.04	J/mol×K	933.14	Joback Method
cpg	714.61	J/mol×K	970.05	Joback Method
cpg	724.55	J/mol×K	1006.95	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=C791355&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume