

2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-5-(o-fluorophenyl)-3-hydroxy

Other names:	2H-1,4-Benzodiazepin-2-one, 7-chloro-5-(2-fluorophenyl)-1,3-dihydro-3-hydroxy- 1,3-Dihydro-7-chloro-5-(o-fluorophenyl)-3-hydroxy-2H-1,4-benzodiazepin-2-one OX 164F RO 7-5205 2H-1,4-Benzodiazepin-2-one, 7-chloro-5-(o-fluorophenyl)-1,3-dihydro-3-hydroxy- N-Desalkyl-3-hydroxyflurazepam 7-Chloro-5-(2-fluorophenyl)-3-hydroxy-1,3-dihydro-2H-1,4-benzodiazepin-2-one Flurazepam, (N-1-des-alkyl, 3-hydroxy) N-1-Desalkyl-3-hydroxyflurazepam CM 40095 3-hydroxy-N-desalkyl-2-oxoquazepam Flurazepam M (N-1-des-alkyl, 3-hydroxy)
Inchi:	InChI=1S/C15H10ClFN2O2/c16-8-5-6-12-10(7-8)13(19-15(21)14(20)18-12)9-3-1-2-4-11(
InchiKey:	FERBACJQVQVCKH-UHFFFAOYSA-N
Formula:	C15H10ClFN2O2
SMILES:	O=C1Nc2ccc(Cl)cc2C(c2ccccc2F)=NC1O
Mol. weight [g/mol]:	304.70
CAS:	17617-60-6

Physical Properties

Property code	Value	Unit	Source
gf	66.57	kJ/mol	Joback Method
hf	-200.49	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	94.19	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.587		Crippen Method
mcvol	200.940	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	929.27	K	Joback Method
tc	1185.50	K	Joback Method
tf	709.51	K	Joback Method
vc	0.765	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.31	J/mol×K	929.27	Joback Method
cpg	609.70	J/mol×K	971.97	Joback Method
cpg	617.46	J/mol×K	1014.68	Joback Method
cpg	623.59	J/mol×K	1057.38	Joback Method
cpg	628.06	J/mol×K	1100.09	Joback Method
cpg	630.88	J/mol×K	1142.79	Joback Method
cpg	632.02	J/mol×K	1185.50	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=C17617606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.cheméo.com/cid/67-575-0/2H-1-4-Benzodiazepin-2-one-1-3-dihydro-7-chloro-5-o-fluorophenyl-3-hydroxy>

Generated by Cheméo on 2024-04-25 04:23:33.242120652 +0000 UTC m=+16308262.162697979.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.