N-1-DESALKYL-3-HYDROXYFLURAZEPAM

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]: 304.71

Physical Properties

Property code	Value	Unit	Source
hfus	41.89	kJ/mol	Joback Method
log10ws	-3.32		Cheméo Relay (1.0)
logp	2.587		Crippen Method
mcvol	200.940	ml/mol	McGowan Method
tf	482.74	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17617606&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point