Norfludiazepam

Other names: 2H-1,4-Benzodiazepin-2-one, 7-chloro-5-(2-fluorophenyl)-1,3-dihydro-
2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-5-(2-fluorophenyl)-
7-Chloro-5-(2-fluorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one
Ro 5-3367
2H-1,4-Benzodiazepin-2-one, 7-chloro-5-(o-fluorophenyl)-1,3-dihydro-
N-Desalkylflutoprazepam
N-Desalkyl-2-oxoquazepam
Dealkylflurazepam
Descarbethoxyloflazepate
N-Desalkylflurazepam
Flurazepam, des-alkyl
Flurazepam M (des-alkyl)
Flurazepam M (N-1-des-alkyl)
N-1-Desalkyl-flurazepam
7-Chloro-5-(o-fluorophenyl)-1,3-dihydro-1,4-benzodiazepin-2-one
Norflutoprazepam
Sch 17514
Desalkylflurazepam
Norfludiazepam - from non-authenticated sample -
7-Chloro-1,3-dihydro-5-(2'-fluorophenyl)-2H-1,4-benzodiazapin-2-one
(desalkylflurazepam)

Inchi: InChI=1S/C15H10ClFN2O/c16-9-5-6-13-11(7-9)15(18-8-14(20)19-13)10-3-1-2-4-12(10)1

InchiKey: UVCOILFBWYKHHB-UHFFFAOYSA-N

Formula: C15H10ClFN2O

SMILES: O=C1CN=C(c2ccccc2F)c2cc(Cl)ccc2N1

Mol. weight [g/mol]: 288.70

CAS: 2886-65-9

Physical Properties

Property code	Value	Unit	Source
gf	211.10	kJ/mol	Joback Method
hf	-27.92	kJ/mol	Joback Method
hfus	36.73	kJ/mol	Joback Method
hvap	77.83	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.269		Crippen Method
mcvol	195.070	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method

rinpol	2457.00		NIST Webbook
rinpol	2475.00		NIST Webbook
rinpol	2442.00		NIST Webbook
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2457.00		NIST Webbook
rinpol	2475.00		NIST Webbook
rinpol	2469.00		NIST Webbook
rinpol	2442.00		NIST Webbook
tb	841.76	K	Joback Method
tc	1121.83	K	Joback Method
tf	652.93	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.33	J/mol×K	1075.15	Joback Method
cpg	551.72	J/mol×K	841.76	Joback Method
cpg	565.08	J/mol×K	888.44	Joback Method
cpg	576.63	J/mol×K	935.12	Joback Method
cpg	586.35	J/mol×K	981.80	Joback Method
cpg	594.25	J/mol×K	1028.47	Joback Method
cpg	604.57	J/mol×K	1121.83	Joback Method
hfust	30.70	kJ/mol	481.20	NIST Webbook

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=C2886659&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
hfust:	Enthalpy of fusion at a given temperature
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