

Hydroxyethylflurazepam

Other names:	3-Hydroxyethylflurazepam
Inchi:	InChI=1S/C17H14ClFN2O2/c18-10-5-6-14-12(9-10)16(11-3-1-2-4-13(11)19)20-15(7-8-22
InchiKey:	JRCYGROYIMMPPPO-UHFFFAOYSA-N
Formula:	C17H14ClFN2O2
SMILES:	O=C1Nc2ccc(Cl)cc2C(c2ccccc2F)=NC1CCO
Mol. weight [g/mol]:	332.76

Physical Properties

Property code	Value	Unit	Source
gf	83.41	kJ/mol	Joback Method
hf	-241.77	kJ/mol	Joback Method
hfus	47.07	kJ/mol	Joback Method
hvap	98.65	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.020		Crippen Method
mcpvol	229.120	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	2630.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	975.03	K	Joback Method
tc	1224.67	K	Joback Method
tf	732.05	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.37	J/molxK	975.03	Joback Method
cpg	721.68	J/molxK	1016.64	Joback Method
cpg	729.30	J/molxK	1058.24	Joback Method
cpg	735.25	J/molxK	1099.85	Joback Method

cpg	739.51	J/mol×K	1141.46	Joback Method
cpg	742.10	J/mol×K	1183.06	Joback Method
cpg	743.01	J/mol×K	1224.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R21813&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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

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