N1-Desalkyl-3-hydroxyflurazepam

Inchi: InChI=1S/C15H10ClFN2O2/c16-9-4-5-12-11(7-9)13(19-15(21)14(20)18-12)8-2-1-3-10(17
InchiKey: FAMAOHPLITWXFB-UHFFFAOYSA-N
Formula: C15H10ClFN2O2
SMILES: O=C1Nc2ccc(Cl)cc2C(c2cccc(F)c2)=NC1O
Mol. weight [g/mol]: 304.70

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
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	929.27	K	Joback Method
tc	1185.50	K	Joback Method
tf	709.51	K	Joback Method
vc	0.765	m3/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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R18133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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