7-Amino-3-hydroxyclonazepam

Inchi: InChI=1S/C16H13ClN2O2/c17-13-4-2-1-3-10(13)11-8-15(20)16(21)19-14-6-5-9(18)7-12(
InchiKey: GPNFJUPJNNKRFV-UHFFFAOYSA-N
Formula: C16H13ClN2O2
SMILES: Nc1ccc2c(c1)C(c1ccccc1Cl)=CC(O)C(=O)N2
Mol. weight [g/mol]: 300.74

Physical Properties

Property code	Value	Unit	Source
gf	219.47	kJ/mol	Joback Method
hf	-62.20	kJ/mol	Joback Method
hfus	41.46	kJ/mol	Joback Method
hvap	101.67	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.667		Crippen Method
mcvol	213.260	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	2890.00		NIST Webbook
tb	971.71	K	Joback Method
tc	1232.54	K	Joback Method
tf	731.91	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.62	J/mol×K	971.71	Joback Method
cpg	643.92	J/mol×K	1015.18	Joback Method
cpg	651.83	J/mol×K	1058.65	Joback Method
cpg	658.38	J/mol×K	1102.12	Joback Method
cpg	663.59	J/mol×K	1145.60	Joback Method
cpg	667.51	J/mol×K	1189.07	Joback Method
cpg	670.14	J/mol×K	1232.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R17430&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