

7-Acetamidoclonazepam

Inchi:	InChI=1S/C17H14ClN3O2/c1-10(22)20-11-6-7-15-13(8-11)17(19-9-16(23)21-15)12-4-2-3
InchiKey:	CSSPKOOFFDJUJC-UHFFFAOYSA-N
Formula:	C17H14ClN3O2
SMILES:	CC(=O)Nc1ccc2c(c1)C(c1ccccc1Cl)=NCC(=O)N2
Mol. weight [g/mol]:	327.76

Physical Properties

Property code	Value	Unit	Source
gf	383.22	kJ/mol	Joback Method
hf	67.80	kJ/mol	Joback Method
hfus	45.53	kJ/mol	Joback Method
hvap	96.28	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.088		Crippen Method
mvol	233.030	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	3263.00		NIST Webbook
rinpol	3263.00		NIST Webbook
tb	992.29	K	Joback Method
tc	1269.36	K	Joback Method
tf	777.47	K	Joback Method
vc	0.882	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.99	J/mol×K	992.29	Joback Method
cpg	719.20	J/mol×K	1038.47	Joback Method
cpg	726.37	J/mol×K	1084.65	Joback Method
cpg	731.50	J/mol×K	1130.82	Joback Method
cpg	734.61	J/mol×K	1177.00	Joback Method
cpg	735.70	J/mol×K	1223.18	Joback Method
cpg	734.79	J/mol×K	1269.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R17412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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