

7-Aminoclonazepam

Other names:

7-Amino-5-(2-chlorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one
Chloraminazepam
Aminoclonazepam
Ro 5-461

Inchi:

2H-1,4-Benzodiazepin-2-one, 7-amino-5-(2-chlorophenyl)-1,3-dihydro-

InchiKey:

HEFRPWRJTGLSSV-UHFFFAOYSA-N

Formula:

C₁₅H₁₂CIN₃O

SMILES:

Nc1ccc2c(c1)C(c1cccc1Cl)=NCC(=O)N2

Mol. weight [g/mol]:

285.73

CAS:

4959-17-5

Physical Properties

Property code	Value	Unit	Source
gf	472.36	kJ/mol	Joback Method
hf	201.98	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	89.28	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.712		Crippen Method
mcvol	203.280	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	2900.00		NIST Webbook
rinpol	2940.20		NIST Webbook
rinpol	2905.00		NIST Webbook
rinpol	2905.00		NIST Webbook
rinpol	2900.00		NIST Webbook
rinpol	2940.20		NIST Webbook
tb	915.02	K	Joback Method
tc	1208.78	K	Joback Method
tf	735.60	K	Joback Method
vc	0.758	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.66	J/mol×K	915.02	Joback Method
cpg	611.30	J/mol×K	963.98	Joback Method
cpg	620.88	J/mol×K	1012.94	Joback Method
cpg	628.41	J/mol×K	1061.90	Joback Method
cpg	633.88	J/mol×K	1110.86	Joback Method
cpg	637.30	J/mol×K	1159.82	Joback Method
cpg	638.66	J/mol×K	1208.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4959175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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