

7-Acetamino-2,3-dihydro-5-phenyl-1H-1,4-benzodiazepin-2-one

Other names:

2H-1,4-Benzodiazepin-2-one, 7-acetamido-1,3-dihydro-5-phenyl-
N-(2-Oxo-5-phenyl-2,3-dihydro-1H-1,4-benzodiazepin-7-yl)acetamide
7-Acetamidonitrazepam
NSC 58777

Inchi: InChI=1S/C17H15N3O2/c1-11(21)19-13-7-8-15-14(9-13)17(18-10-16(22)20-15)12-5-3-2**InchiKey:** JHTJXLGLYZQIGI-UHFFFAOYSA-N**Formula:** C17H15N3O2**SMILES:** CC(=O)Nc1ccc2c(c1)C(c1ccccc1)=NCC(=O)N2**Mol. weight [g/mol]:** 293.32**CAS:** 4928-03-4

Physical Properties

Property code	Value	Unit	Source
gf	404.78	kJ/mol	Joback Method
hf	95.01	kJ/mol	Joback Method
hfus	41.72	kJ/mol	Joback Method
hvap	91.23	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.434		Crippen Method
mcvol	220.790	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	3205.00		NIST Webbook
rinpol	3205.00		NIST Webbook
tb	949.88	K	Joback Method
tc	1225.29	K	Joback Method
tf	735.03	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.13	J/molxK	949.88	Joback Method
cpg	705.50	J/molxK	995.78	Joback Method
cpg	714.84	J/molxK	1041.68	Joback Method

cpg	722.17	J/mol×K	1087.58	Joback Method
cpg	727.51	J/mol×K	1133.48	Joback Method
cpg	730.89	J/mol×K	1179.39	Joback Method
cpg	732.31	J/mol×K	1225.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4928034&Units=SI

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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