7-ACETAMINO-2,3-DIHYDRO-5-PHENYL-1H-1,4-BI

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]: 293.33

Physical Properties

Property code	Value	Unit	Source
hfus	41.72	kJ/mol	Joback Method
log10ws	-3.17		Cheméo Relay (1.0)
logp	2.434		Crippen Method
mcvol	220.790	ml/mol	McGowan Method
rinpol	3205.00		NIST Webbook
rinpol	3205.00		NIST Webbook
tf	513.51	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4928034&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point