7-Amino-2,3-dihydro-5-phenyl-1H-1,4-benzodiaze

Other names: 7-Aminonitrazepam
Inchi: InChI=1S/C15H13N3O/c16-11-6-7-13-12(8-11)15(17-9-14(19)18-13)10-4-2-1-3-5-10/h1-
InchiKey: OYOUQHVDCKOOAL-UHFFFAOYSA-N
Formula: C15H13N3O
SMILES: Nc1ccc2c(c1)C(c1ccccc1)=NCC(O)=N2
Mol. weight [g/mol]: 251.28
CAS: 4928-02-3

Physical Properties

Property code	Value	Unit	Source
gf	529.09	kJ/mol	Joback Method
hf	294.13	kJ/mol	Joback Method
hfus	36.00	kJ/mol	Joback Method
hvap	97.07	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.708		Crippen Method
mcvol	191.040	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpol	2898.70		NIST Webbook
rinpol	2785.00		NIST Webbook
rinpol	2898.70		NIST Webbook
rinpol	2785.00		NIST Webbook
rinpol	2785.00		NIST Webbook
tb	906.26	K	Joback Method
tc	1170.13	K	Joback Method
tf	665.55	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.79	J/mol×K	906.26	Joback Method
cpg	611.59	J/mol×K	950.24	Joback Method
cpg	620.84	J/mol×K	994.22	Joback Method

cpg	628.59	J/mol×K	1038.20	Joback Method
cpg	634.88	J/mol×K	1082.17	Joback Method
cpg	639.77	J/mol×K	1126.15	Joback Method
cpg	643.31	J/mol×K	1170.13	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=C4928023&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