1-(N-Benzyl-N-acetyl)amino-6-(2-cyanoethyl)cyclo

Inchi: InChI=1S/C18H22N2O/c1-15(21)20(14-16-8-3-2-4-9-16)18-12-6-5-10-17(18)11-7-13-19/
InchiKey: LXYILFDQWXGWHI-UHFFFAOYSA-N
Formula: C18H22N2O
SMILES: CC(=O)N(Cc1ccccc1)C1=CCCCC1CCC#N
Mol. weight [g/mol]: 282.38
CAS: 82365-22-8

Physical Properties

Property code	Value	Unit	Source
gf	372.91	kJ/mol	Joback Method
hf	42.14	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	78.59	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.023		Crippen Method
mcvol	238.490	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
tb	830.00	K	Joback Method
tc	1061.70	K	Joback Method
tf	487.09	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.77	J/mol×K	830.00	Joback Method
cpg	739.44	J/mol×K	868.62	Joback Method
cpg	753.83	J/mol×K	907.23	Joback Method
cpg	767.04	J/mol×K	945.85	Joback Method
cpg	779.13	J/mol×K	984.47	Joback Method
cpg	790.20	J/mol×K	1023.09	Joback Method
cpg	800.33	J/mol×K	1061.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82365228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume