

trans-1,4-Diacetamidocyclohexane

Other names:	Acetamide, N,N'-1,4-cyclohexanediylbis-, trans-Acetamide, N,N'-1,4-cyclohexylenebis-, trans-Acetamide, n,n'-(p-cyclohexylene)bis-, trans-N-[4-(Acetylamino)cyclohexyl]acetamide, (E)-
Inchi:	InChI=1S/C10H18N2O2/c1-7(13)11-9-3-5-10(6-4-9)12-8(2)14/h9-10H,3-6H2,1-2H3,(H,1
InchiKey:	TVILGUBKPIUIFC-MGCOHNPYSA-N
Formula:	C10H18N2O2
SMILES:	CC(=O)NC1CCC(NC(C)=O)CC1
Mol. weight [g/mol]:	198.26
CAS:	2077-92-1

Physical Properties

Property code	Value	Unit	Source
gf	-29.00	kJ/mol	Joback Method
hf	-333.97	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	64.34	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	0.570		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	651.16	K	Joback Method
tc	866.10	K	Joback Method
tf	410.78	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.21	J/molxK	651.16	Joback Method
cpg	477.66	J/molxK	686.98	Joback Method
cpg	493.04	J/molxK	722.81	Joback Method
cpg	507.38	J/molxK	758.63	Joback Method
cpg	520.71	J/molxK	794.45	Joback Method

cpg	533.04	J/mol×K	830.27	Joback Method
cpg	544.41	J/mol×K	866.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2077921&Units=SI
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

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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