

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)N[C@H]1CC[C@H](NC(C)=O)CC1
Mol. weight [g/mol]:	198.27

Physical Properties

Property code	Value	Unit	Source
hfus	27.96	kJ/mol	Joback Method
log10ws	-1.46		Cheméo Relay (1.0)
logp	0.570		Crippen Method
mcvol	164.000	ml/mol	McGowan Method

Temperature Dependent Properties

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2077921&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

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

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