

N-Tricyclo[3.3.1.1[3,7]]dec-2-ylacetamide

Inchi:	InChI=1S/C12H19NO/c1-7(14)13-12-10-3-8-2-9(5-10)6-11(12)4-8/h8-12H,2-6H2,1H3,(H,
InchiKey:	OFEZUSBZKMXQEU-UHFFFAOYSA-N
Formula:	C12H19NO
SMILES:	CC(=O)NC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]:	193.29

Physical Properties

Property code	Value	Unit	Source
hfus	27.98	kJ/mol	Joback Method
logp	1.947		Crippen Method
mcvol	158.910	ml/mol	McGowan Method
rinpol	1761.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.59	J/mol×K	593.15	Joback Method
cpg	475.34	J/mol×K	629.20	Joback Method
cpg	493.76	J/mol×K	665.26	Joback Method
cpg	510.94	J/mol×K	701.31	Joback Method
cpg	526.99	J/mol×K	737.36	Joback Method
cpg	541.99	J/mol×K	773.42	Joback Method
cpg	556.06	J/mol×K	809.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52917723&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):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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