

CYCLO-(L-VALYL-L-PHENYLALANYL)

Other names:	3-Benzyl-6-isopropyl-2,5-piperazinedione
Inchi:	InChI=1S/C14H18N2O2/c1-9(2)12-14(18)15-11(13(17)16-12)8-10-6-4-3-5-7-10/h3-7,9,11
InchiKey:	OQQPOHUVAQPSHJ-UHFFFAOYSA-N
Formula:	C14H18N2O2
SMILES:	CC(C)C1NC(=O)C(Cc2ccccc2)NC1=O
Mol. weight [g/mol]:	246.31

Physical Properties

Property code	Value	Unit	Source
chs	-7689.00 ± 4.00	kJ/mol	NIST Webbook
hfus	33.64	kJ/mol	Joback Method
logp	0.868		Crippen Method
mcvol	196.600	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.92	J/mol×K	793.58	Joback Method
cpg	624.60	J/mol×K	837.43	Joback Method
cpg	641.30	J/mol×K	881.28	Joback Method
cpg	655.95	J/mol×K	925.13	Joback Method
cpg	668.49	J/mol×K	968.98	Joback Method
cpg	678.85	J/mol×K	1012.83	Joback Method
cpg	686.97	J/mol×K	1056.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14474716&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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