

# D-Val, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi:	InChI=1S/C16H24N2O3/c1-5-21-16(20)18-14(11(2)3)15(19)17-12(4)13-9-7-6-8-10-13/h6
InchiKey:	GPURSIJORGZPY-GXTWGEZSA-N
Formula:	C16H24N2O3
SMILES:	CCOC(=O)NC(C(=O)NC(C)c1ccccc1)C(C)C
Mol. weight [g/mol]:	292.37

## Physical Properties

Property code	Value	Unit	Source
gf	4.87	kJ/mol	Joback Method
hf	-403.32	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.634		Crippen Method
mvol	241.510	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2093.00		NIST Webbook
tb	821.34	K	Joback Method
tc	1034.39	K	Joback Method
tf	478.91	K	Joback Method
vc	0.905	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.56	J/molxK	821.34	Joback Method
cpg	750.20	J/molxK	856.85	Joback Method
cpg	763.71	J/molxK	892.36	Joback Method
cpg	776.13	J/molxK	927.86	Joback Method
cpg	787.51	J/molxK	963.37	Joback Method
cpg	797.88	J/molxK	998.88	Joback Method
cpg	807.29	J/molxK	1034.39	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R587538&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R587538&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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