

Valdetamide

Other names:	4-Pentenamide, 2,2-diethyl-Diethylallylacetamide Epinoval Novonal 2,2-Diethyl-4-pentenamide Allyldiethylacetamide
Inchi:	InChI=1S/C9H17NO/c1-4-7-9(5-2,6-3)8(10)11/h4H,1,5-7H2,2-3H3,(H2,10,11)
InchiKey:	LOMDVEFCNVDZMZ-UHFFFAOYSA-N
Formula:	C9H17NO
SMILES:	<chem>C=CCC(CC)(CC)C(N)=O</chem>
Mol. weight [g/mol]:	155.24
CAS:	512-48-1

Physical Properties

Property code	Value	Unit	Source
gf	53.11	kJ/mol	Joback Method
hf	-191.20	kJ/mol	Joback Method
hfus	17.17	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.854		Crippen Method
mvol	144.920	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	525.17	K	Joback Method
tc	725.23	K	Joback Method
tf	325.04	K	Joback Method
vc	0.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.62	J/mol×K	525.17	Joback Method

cpg	357.66	J/mol×K	558.51	Joback Method
cpg	370.87	J/mol×K	591.86	Joback Method
cpg	383.29	J/mol×K	625.20	Joback Method
cpg	394.97	J/mol×K	658.54	Joback Method
cpg	405.95	J/mol×K	691.88	Joback Method
cpg	416.27	J/mol×K	725.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C512481&Units=SI

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

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