

Valerenal

Inchi:	InChI=1S/C15H22O/c1-10(9-16)8-13-6-4-11(2)14-7-5-12(3)15(13)14/h8-9,11,13-14H,4-7
InchiKey:	RJZWGDPBGWGJNU-CSKARUKUSA-N
Formula:	C15H22O
SMILES:	CC(C=O)=CC1CCC(C)C2CCC(C)=C12
Mol. weight [g/mol]:	218.33
CAS:	4176-16-3

Physical Properties

Property code	Value	Unit	Source
gf	135.76	kJ/mol	Joback Method
hf	-189.46	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	57.39	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1668.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1715.70		NIST Webbook
rinpol	1727.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2207.00		NIST Webbook
ripol	2207.00		NIST Webbook
tb	626.04	K	Joback Method
tc	843.09	K	Joback Method
tf	328.65	K	Joback Method
vc	0.749	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.96	J/mol×K	626.04	Joback Method

cpg	550.05	J/mol×K	662.22	Joback Method
cpg	568.90	J/mol×K	698.39	Joback Method
cpg	586.58	J/mol×K	734.57	Joback Method
cpg	603.16	J/mol×K	770.74	Joback Method
cpg	618.71	J/mol×K	806.92	Joback Method
cpg	633.30	J/mol×K	843.09	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=C4176163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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