Valerenic acid

Other names:	2-Propenoic acid, 3-[(4S,7R,7aR)-2,4,5,6,7,7a-hexahydro-3,7-dimethyl-1H-inden-4-yl]-2-methyl-, (2E)- Valeric acid
Inchi:	InChI=1S/C15H22O2/c1-9-4-6-12(8-11(3)15(16)17)14-10(2)5-7-13(9)14/h8-9,12-13H,4-7
InchiKey:	FEBNTWHYQKGEIQ-OPZDXMJLSA-N
Formula:	C15H22O2
SMILES:	CC(=CC1CCC(C)C2CCC(C)=C12)C(=O)O
Mol. weight [g/mol]:	234.33
CAS:	3569-10-6

Physical Properties

Property code	Value	Unit	Source
gf	-30.46	kJ/mol	Joback Method
hf	-368.69	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	74.10	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.790		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1876.50		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1862.50		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1831.00		NIST Webbook
tb	723.43	K	Joback Method
tc	930.48	K	Joback Method
tf	397.40	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.59	J/mol×K	723.43	Joback Method
cpg	613.04	J/mol×K	757.94	Joback Method

cpg	628.50	J/mol×K	792.45	Joback Method
cpg	643.03	J/mol×K	826.95	Joback Method
cpg	656.70	J/mol×K	861.46	Joback Method
cpg	669.56	J/mol×K	895.97	Joback Method
cpg	681.69	J/mol×K	930.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3569106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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