Valerianol acetate

Inchi: InChI=1S/C17H28O2/c1-12-7-6-8-14-9-10-15(11-17(12,14)5)16(3,4)19-13(2)18/h8,12,15
InchiKey: KWFVLNZOTCEVEH-YLQAJVPDSA-N
Formula: C17H28O2
SMILES: CC(=O)OC(C)(C)C1CCC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-58.59	kJ/mol	Joback Method
hf	-485.59	kJ/mol	Joback Method
hfus	18.64	kJ/mol	Joback Method
hvap	61.30	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.491		Crippen Method
mcvol	231.810	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	1925.00		NIST Webbook
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tb	691.69	K	Joback Method
tc	916.62	K	Joback Method
tf	410.67	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.68	J/mol×K	691.69	Joback Method
cpg	716.12	J/mol×K	729.18	Joback Method
cpg	737.32	J/mol×K	766.67	Joback Method
cpg	757.44	J/mol×K	804.16	Joback Method
cpg	776.66	J/mol×K	841.65	Joback Method
cpg	795.13	J/mol×K	879.14	Joback Method
cpg	813.02	J/mol×K	916.62	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=R417904&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume