Valerianol (Khusunol)

Inchi: InChI=1S/C15H24O/c1-10-13-5-4-12(9-16)15(13)7-6-11(8-15)14(10,2)3/h11-13,16H,1,4-
InchiKey: OOYRHNIVDZZGQV-PWNZVWSESA-N
Formula: C15H24O
SMILES: C=C1C2CCC(CO)C23CCC(C3)C1(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	123.33	kJ/mol	Joback Method
hf	-225.04	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	62.98	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.387		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1623.00		NIST Webbook
rinpol	1626.00		NIST Webbook
tb	653.84	K	Joback Method
tc	861.60	K	Joback Method
tf	419.41	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.73	J/mol×K	653.84	Joback Method
cpg	592.34	J/mol×K	688.47	Joback Method
cpg	610.14	J/mol×K	723.09	Joback Method
cpg	627.34	J/mol×K	757.72	Joback Method
cpg	644.19	J/mol×K	792.34	Joback Method
cpg	660.92	J/mol×K	826.97	Joback Method
cpg	677.76	J/mol×K	861.60	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=R613157&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

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