

Valerianol

Other names:	valeranol
Inchi:	InChI=1S/C15H26O/c1-11-6-5-7-12-8-9-13(14(2,3)16)10-15(11,12)4/h7,11,13,16H,5-6,8
InchiKey:	MQWIFDHBNGIVPO-CORIIIEPSA-N
Formula:	C15H26O
SMILES:	CC1CCC=C2CCC(C(C)(C)O)CC21C
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
hfus	14.76	kJ/mol	Joback Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1650.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1648.20		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1653.00		NIST Webbook

rinpol	1651.00	NIST Webbook
rinpol	1655.00	NIST Webbook
rinpol	1644.00	NIST Webbook
rinpol	1640.00	NIST Webbook
ripol	2215.00	NIST Webbook
ripol	2208.00	NIST Webbook
ripol	2205.00	NIST Webbook
ripol	2231.00	NIST Webbook
ripol	2215.00	NIST Webbook
ripol	2208.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.13	J/mol×K	661.82	Joback Method
cpg	618.08	J/mol×K	697.19	Joback Method
cpg	636.92	J/mol×K	732.57	Joback Method
cpg	654.81	J/mol×K	767.94	Joback Method
cpg	671.91	J/mol×K	803.32	Joback Method
cpg	688.38	J/mol×K	838.69	Joback Method
cpg	704.35	J/mol×K	874.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199334&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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