

Valerianol

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,5-6,8H
InchiKey:	MQWIFDHBNGIVPO-LKVSRLFHLSA-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	1655.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1610.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R612763&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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):

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

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