

Fukinone

Inchi:	InChI=1S/C15H24O/c1-10(2)13-9-15(4)11(3)6-5-7-12(15)8-14(13)16/h11-12H,5-9H2,1-4H
InchiKey:	HMLGXKHWABZSIS-XUJVEKNSA-N
Formula:	C15H24O
SMILES:	CC(C)=C1CC2(C)C(C)CCCC2CC1=O
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
hfus	15.77	kJ/mol	Joback Method
hvap	71.55	kJ/mol	Cheméo Relay (1.0)
logp	4.128		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1756.00		NIST Webbook
ripol	2254.00		NIST Webbook
tb	570.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.44	J/mol×K	643.07	Joback Method
cpg	586.66	J/mol×K	682.53	Joback Method
cpg	608.57	J/mol×K	721.99	Joback Method
cpg	629.33	J/mol×K	761.45	Joback Method
cpg	649.07	J/mol×K	800.91	Joback Method
cpg	667.95	J/mol×K	840.37	Joback Method
cpg	686.13	J/mol×K	879.83	Joback Method

Sources

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=R616116&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/ci990307I>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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