

khusinol

Inchi:	InChI=1S/C15H24O/c1-9(2)12-6-5-11(4)15-13(12)7-10(3)8-14(15)16/h7,9,12-16H,4-6,8H
InchiKey:	WFHKESPONQXPGD-FEWQNLEASA-N
Formula:	C15H24O
SMILES:	C=C1CCC(C(C)C)C2C=C(C)CC(O)C12
Mol. weight [g/mol]:	220.35
CAS:	24268-34-6

Physical Properties

Property code	Value	Unit	Source
gf	67.25	kJ/mol	Joback Method
hf	-299.61	kJ/mol	Joback Method
hfus	24.86	kJ/mol	Joback Method
hvap	66.28	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.552		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1674.00		NIST Webbook

rinpol	1674.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1664.00		NIST Webbook
tb	658.86	K	Joback Method
tc	858.82	K	Joback Method
tf	344.91	K	Joback Method
vc	0.739	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.43	J/molxK	658.86	Joback Method
cpg	596.53	J/molxK	692.19	Joback Method
cpg	614.55	J/molxK	725.51	Joback Method
cpg	631.52	J/molxK	758.84	Joback Method
cpg	647.47	J/molxK	792.17	Joback Method
cpg	662.43	J/molxK	825.50	Joback Method
cpg	676.45	J/molxK	858.82	Joback Method
dvisc	0.0046470	Paxs	344.91	Joback Method
dvisc	0.0017837	Paxs	397.24	Joback Method
dvisc	0.0008556	Paxs	449.56	Joback Method
dvisc	0.0004784	Paxs	501.88	Joback Method
dvisc	0.0002985	Paxs	554.21	Joback Method
dvisc	0.0002020	Paxs	606.54	Joback Method
dvisc	0.0001455	Paxs	658.86	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=C24268346&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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