

Kunzeaol

Inchi:	InChI=1S/C15H26O/c1-11(2)14-9-8-12(3)6-5-7-13(4)10-15(14)16/h6,10-11,14-16H,5,7-9
InchiKey:	PXMCURAOQSNMOZ-ZDYWMRFRSA-N
Formula:	C15H26O
SMILES:	CC1=CC(O)C(C(C)C)CCC(C)=CCC1
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	-54.84	kJ/mol	Joback Method
hf	-408.48	kJ/mol	Joback Method
hfus	21.34	kJ/mol	Joback Method
hvap	67.99	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.086		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
ripol	1705.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	2326.00		NIST Webbook
ripol	2326.00		NIST Webbook
tb	674.58	K	Joback Method
tc	881.07	K	Joback Method
tf	320.25	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.13	J/molxK	674.58	Joback Method
cpg	619.44	J/molxK	708.99	Joback Method
cpg	638.54	J/molxK	743.41	Joback Method
cpg	656.42	J/molxK	777.82	Joback Method
cpg	673.09	J/molxK	812.24	Joback Method
cpg	688.54	J/molxK	846.65	Joback Method

cpg	702.77	J/molxK	881.07	Joback Method
dvisc	0.0102052	Paxs	320.25	Joback Method
dvisc	0.0015204	Paxs	379.31	Joback Method
dvisc	0.0003783	Paxs	438.36	Joback Method
dvisc	0.0001310	Paxs	497.41	Joback Method
dvisc	0.0000568	Paxs	556.47	Joback Method
dvisc	0.0000289	Paxs	615.52	Joback Method
dvisc	0.0000166	Paxs	674.58	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=R285980&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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