(-)-Kessane

Inchi: InChI=1S/C14H24O/c1-9-5-6-12-11(9)7-10-8-14(12,4)15-13(10,2)3/h9-12H,5-8H2,1-4H3
InchiKey: WBHXSKHCVPVDDZ-JNLQPACOSA-N
Formula: C14H24O
SMILES: CC1CCC2C1CC1CC2(C)OC1(C)C
Mol. weight [g/mol]: 208.34

Physical Properties

Property code	Value	Unit	Source
gf	104.82	kJ/mol	Joback Method
hf	-288.75	kJ/mol	Joback Method
hfus	20.82	kJ/mol	Joback Method
hvap	48.12	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.626		Crippen Method
mcvol	181.410	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	561.90	K	Joback Method
tc	785.89	K	Joback Method
tf	355.97	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.44	J/mol×K	561.90	Joback Method
cpg	530.02	J/mol×K	599.23	Joback Method
cpg	551.98	J/mol×K	636.56	Joback Method
cpg	572.60	J/mol×K	673.90	Joback Method
cpg	592.17	J/mol×K	711.23	Joback Method
cpg	610.96	J/mol×K	748.56	Joback Method
cpg	629.26	J/mol×K	785.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R412018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg:	Ideal gas heat capacity
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