Kessyl alcohol

Inchi: InChI=1S/C15H26O2/c1-9-7-12(16)13-11(9)8-10-5-6-15(13,4)17-14(10,2)3/h9-13,16H,5-
InchiKey: ZADVMZUKWWMSLQ-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: CC1CC(O)C2C1CC1CCC2(C)OC1(C)C
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-43.39	kJ/mol	Joback Method
hf	-488.12	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	66.89	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.987		Crippen Method
mcvol	201.370	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1690.20		NIST Webbook
rinpol	1662.00		NIST Webbook
tb	676.56	K	Joback Method
tc	887.16	K	Joback Method
tf	420.30	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.59	J/mol×K	676.56	Joback Method
cpg	659.20	J/mol×K	711.66	Joback Method
cpg	678.97	J/mol×K	746.76	Joback Method
cpg	698.13	J/mol×K	781.86	Joback Method
cpg	716.90	J/mol×K	816.96	Joback Method
cpg	735.51	J/mol×K	852.06	Joback Method
cpg	754.18	J/mol×K	887.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341045&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