((3S,3aR,6R,8aS)-7,7-Dimethyl-8-methyleneoctahy

Other names: Khusimol
Khusenol
Tricyclovetivenol
Zizanol

Inchi: InChI=1S/C15H24O/c1-10-13-5-4-12(9-16)15(13)7-6-11(8-15)14(10,2)3/h11-13,16H,1,4-

InchiKey: OOYRHNIVDZZGQV-OCLBVPJSSA-N

Formula: C15H24O

SMILES: C=C1C2CCC(CO)C23CCC(C3)C1(C)C

Mol. weight [g/mol]: 220.35

CAS: 16223-63-5

Physical Properties

Property code	Value	Unit	Source
gf	123.33	kJ/mol	Joback Method
hf	-225.04	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	62.98	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.387		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1743.00		NIST Webbook
ripol	2521.00		NIST Webbook
tb	653.84	K	Joback Method
tc	861.60	K	Joback Method
tf	419.41	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.73	J/mol×K	653.84	Joback Method
cpg	592.34	J/mol×K	688.47	Joback Method
cpg	610.14	J/mol×K	723.09	Joback Method
cpg	627.34	J/mol×K	757.72	Joback Method
cpg	644.19	J/mol×K	792.34	Joback Method
cpg	660.92	J/mol×K	826.97	Joback Method
cpg	677.76	J/mol×K	861.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16223635&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume