2-((2R,8R,8aS)-8,8a-Dimethyl-1,2,3,4,6,7,8,8a-octal

Other names:	Valerianol Kusenol Kusunol 2-Naphthalenemethanol, 1,2,3,4,6,7,8,8a-octahydro-«alpha»,«alpha»,8,8a-tetramethyl-, (2R,8R,8aS)-
Inchi:	InChI=1S/C15H26O/c1-11-6-5-7-12-8-9-13(14(2,3)16)10-15(11,12)4/h7,11,13,16H,5-6,8-
InchiKey:	MQWIFDHBNGIVPO-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	CC1CCC=C2CCC(C(C)(C)O)CC21C
Mol. weight [g/mol]:	222.37
CAS:	20489-45-6

Physical Properties

Property code	Value	Unit	Source
gf	21.67	kJ/mol	Joback Method
hf	-351.74	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1661.00		NIST Webbook
rinpol	1661.00		NIST Webbook
tb	661.82	K	Joback Method
tc	874.07	K	Joback Method
tf	376.79	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.13	J/mol×K	661.82	Joback Method
cpg	618.08	J/mol×K	697.19	Joback Method
cpg	636.92	J/mol×K	732.57	Joback Method

cpg	654.81	J/mol×K	767.94	Joback Method
cpg	671.91	J/mol×K	803.32	Joback Method
cpg	688.38	J/mol×K	838.69	Joback Method
cpg	704.35	J/mol×K	874.07	Joback Method

Sources

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=C20489456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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