

2-((2R,4aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydro

Inchi:	InChI=1S/C15H24O/c1-11-5-4-7-15(3)8-6-13(9-14(11)15)12(2)10-16/h13,16H,2,4-10H2,
InchiKey:	ITRHZWKEZJYJQO-ZFWWWQNUSA-N
Formula:	C15H24O
SMILES:	C=C(CO)C1CCC2(C)CCCC(C)=C2C1
Mol. weight [g/mol]:	220.35
CAS:	65018-14-6

Physical Properties

Property code	Value	Unit	Source
gf	96.20	kJ/mol	Joback Method
hf	-218.48	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	66.05	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.842		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1752.30		NIST Webbook
tb	671.26	K	Joback Method
tc	880.48	K	Joback Method
tf	375.41	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.97	J/mol×K	671.26	Joback Method
cpg	588.24	J/mol×K	706.13	Joback Method
cpg	605.61	J/mol×K	741.00	Joback Method
cpg	622.21	J/mol×K	775.87	Joback Method
cpg	638.18	J/mol×K	810.74	Joback Method
cpg	653.65	J/mol×K	845.61	Joback Method
cpg	668.76	J/mol×K	880.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C65018146&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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