

(3aR,4aS,5R,9aS)-5,8-Dimethyl-3-methylene-3a,4,4a,8a-tetrahydronaphthalene

Inchi:	InChI=1S/C15H20O2/c1-8-4-5-11-9(2)6-14-13(7-12(8)11)10(3)15(16)17-14/h8,12-14H,3
InchiKey:	GAPVTYWDGWKUKK-UHFFFAOYSA-N
Formula:	C15H20O2
SMILES:	C=C1C(=O)OC2CC(C)=C3CCC(C)C3CC12
Mol. weight [g/mol]:	232.32
CAS:	66873-37-8

Physical Properties

Property code	Value	Unit	Source
gf	56.63	kJ/mol	Joback Method
hf	-330.13	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.241		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1967.10		NIST Webbook
rinpol	1948.00		NIST Webbook
tb	678.28	K	Joback Method
tc	913.85	K	Joback Method
tf	428.58	K	Joback Method
vc	0.712	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.96	J/molxK	678.28	Joback Method
cpg	583.85	J/molxK	717.54	Joback Method
cpg	603.34	J/molxK	756.80	Joback Method
cpg	621.47	J/molxK	796.06	Joback Method
cpg	638.29	J/molxK	835.33	Joback Method
cpg	653.85	J/molxK	874.59	Joback Method
cpg	668.18	J/molxK	913.85	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=C66873378&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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