

(3S,3aS,6R,7R,9aS)-1,1,7-Trimethyldecahydro-3a,

Inchi:	InChI=1S/C15H26O2/c1-13(2)8-12(17)15-7-5-11(16)14(3,9-15)6-4-10(13)15/h10-12,16-1
InchiKey:	BWXJQHJHGMZLBT-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	CC1(C)CC(O)C23CCC(O)C(C)(CCC12)C3
Mol. weight [g/mol]:	238.37
CAS:	2649-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-91.87	kJ/mol	Joback Method
hf	-472.77	kJ/mol	Joback Method
hfus	15.21	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.725		Crippen Method
mvol	201.370	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1885.20		NIST Webbook
rinpol	1885.20		NIST Webbook
tb	746.70	K	Joback Method
tc	953.16	K	Joback Method
tf	482.69	K	Joback Method
vc	0.751	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.30	J/molxK	746.70	Joback Method
cpg	685.84	J/molxK	781.11	Joback Method
cpg	704.43	J/molxK	815.52	Joback Method
cpg	723.35	J/molxK	849.93	Joback Method
cpg	742.89	J/molxK	884.34	Joback Method
cpg	763.36	J/molxK	918.75	Joback Method
cpg	785.05	J/molxK	953.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2649641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
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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