(+)-(1S,3aR,7S,7aR)-2,3,3a,4,5,6,7,7a-Octahydro-7,

Inchi: InChI=1S/C15H28O/c1-10(2)14(16)13-9-8-12-7-5-6-11(3)15(12,13)4/h10-14,16H,5-9H2,1
InchiKey: OLSZYGCUKSYWHW-YKYMWBLQSA-N
Formula: C15H28O
SMILES: CC(C)C(O)C1CCC2CCCC(C)C21C
Mol. weight [g/mol]: 224.38

Physical Properties

Property code	Value	Unit	Source
gf	-1.99	kJ/mol	Joback Method
hf	-414.04	kJ/mol	Joback Method
hfus	17.46	kJ/mol	Joback Method
hvap	63.46	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.856		Crippen Method
mcvol	206.360	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1645.00		NIST Webbook
tb	651.09	K	Joback Method
tc	851.50	K	Joback Method
tf	330.37	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.09	J/mol×K	651.09	Joback Method
cpg	638.74	J/mol×K	684.49	Joback Method
cpg	658.35	J/mol×K	717.89	Joback Method
cpg	677.02	J/mol×K	751.29	Joback Method
cpg	694.88	J/mol×K	784.70	Joback Method
cpg	712.04	J/mol×K	818.10	Joback Method
cpg	728.62	J/mol×K	851.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R281557&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

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