

(3R,3aR,5S,6R,7aR)-3,6,7,7-Tetramethyloctahydro

Inchi:	InChI=1S/C15H26O/c1-10-5-6-11-13(2,3)14(4)7-8-15(10,11)9-12(14)16/h10-12,16H,5-9H
InchiKey:	CSTOJISGDOIIDQ-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	CC1CCC2C13CCC(C)(C(O)C3)C2(C)C
Mol. weight [g/mol]:	222.37
CAS:	50657-30-2

Physical Properties

Property code	Value	Unit	Source
gf	57.05	kJ/mol	Joback Method
hf	-314.38	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	61.37	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.610		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1598.80		NIST Webbook
rinpol	1615.00		NIST Webbook
rinpol	1598.80		NIST Webbook
rinpol	1615.00		NIST Webbook
tb	650.25	K	Joback Method
tc	863.66	K	Joback Method
tf	425.39	K	Joback Method
vc	0.741	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.75	J/mol×K	650.25	Joback Method
cpg	615.74	J/mol×K	685.82	Joback Method
cpg	634.97	J/mol×K	721.39	Joback Method
cpg	653.76	J/mol×K	756.96	Joback Method
cpg	672.45	J/mol×K	792.52	Joback Method

cpg	691.37	J/mol×K	828.09	Joback Method
cpg	710.84	J/mol×K	863.66	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=C50657302&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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