

TETRACYCLO[6.3.2.0(2,5).0(1,8)]TRIDECAN-9-OL, 4,4-DIMETHYL-

Other names:	4,4-Dimethyltetracyclo-(6,3,2,0)(2,5)0(1,8)tridecan-9-ol
Inchi:	InChI=1S/C15H24O/c1-13(2)9-11-10(13)3-5-15-8-7-14(11,15)6-4-12(15)16/h10-12,16H,3
InchiKey:	DFBIFSIVSFAGEV-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC1(C)CC2C1CCC13CCC21CCC3O
Mol. weight [g/mol]:	220.36

Physical Properties

Property code	Value	Unit	Source
hfus	12.38	kJ/mol	Joback Method
logp	3.364		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
ripol	2257.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.25	J/mol×K	657.39	Joback Method
cpg	596.52	J/mol×K	694.17	Joback Method
cpg	615.08	J/mol×K	730.95	Joback Method
cpg	633.33	J/mol×K	767.72	Joback Method
cpg	651.68	J/mol×K	804.50	Joback Method
cpg	670.55	J/mol×K	841.28	Joback Method
cpg	690.36	J/mol×K	878.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U157751&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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