

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]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	137.61	kJ/mol	Joback Method
hf	-215.08	kJ/mol	Joback Method
hfus	12.38	kJ/mol	Joback Method
hvap	61.42	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.364		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
ripol	2257.00		NIST Webbook
tb	657.39	K	Joback Method
tc	878.06	K	Joback Method
tf	451.09	K	Joback Method
vc	0.707	m ³ /kmol	Joback Method

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

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=U157751&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
ri pol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/59-565-0/Tetracyclo-6-3-2-0-2-5-0-1-8-tridecan-9-ol-4-4-dimethyl.pdf>

Generated by Cheméo on 2024-05-03 13:24:30.077266975 +0000 UTC m=+17031918.997844297.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.