

Tricyclo[2.2.1.0^{2,6}]heptane-3-methanol, 2,3-dimethyl-

Other names:	Teresantalol
	Tricyclo[2.2.1.0(2,6)]heptane-3-methanol, 2,3-dimethyl-, stereoisomer
Inchi:	InChI=1S/C10H16O/c1-9(5-11)6-3-7-8(4-6)10(7,9)2/h6-8,11H,3-5H2,1-2H3
InchiKey:	ZWUWJJHLJNLVDD-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1(CO)C2CC3C(C2)C31C
Mol. weight [g/mol]:	152.24

Physical Properties

Property code	Value	Unit	Source
hfus	13.89	kJ/mol	Joback Method
logp	1.661		Crippen Method
mcvol	125.050	ml/mol	McGowan Method
rinpol	1286.00		NIST Webbook
tb	484.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.09	J/mol×K	523.20	Joback Method
cpg	353.37	J/mol×K	555.61	Joback Method
cpg	366.45	J/mol×K	588.03	Joback Method
cpg	378.55	J/mol×K	620.44	Joback Method
cpg	389.87	J/mol×K	652.86	Joback Method
cpg	400.62	J/mol×K	685.27	Joback Method
cpg	411.01	J/mol×K	717.68	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C29550558&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>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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