

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]:	152.23
CAS:	29550-55-8

Physical Properties

Property code	Value	Unit	Source
gf	76.55	kJ/mol	Joback Method
hf	-181.44	kJ/mol	Joback Method
hfus	13.89	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.661		Crippen Method
mvol	125.050	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1286.00		NIST Webbook
tb	523.20	K	Joback Method
tc	717.68	K	Joback Method
tf	363.46	K	Joback Method
vc	0.495	m ³ /kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29550558&Units=SI
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

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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