

trans-«alpha»,«alpha»,5-Trimethyl-5-ethenyltetrahydropyran

Inchi:	InChI=1S/C10H18O2/c1-5-10(4)7-6-8(12-10)9(2,3)11/h5,8,11H,1,6-7H2,2-4H3/t8-,10+/m
InchiKey:	BRHDDEIRQPDPMG-SCZZXKLOSA-N
Formula:	C10H18O2
SMILES:	C=CC1(C)CCC(C(C)(C)O)O1
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
hfus	13.74	kJ/mol	Joback Method
logp	1.881		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.75	J/mol×K	551.63	Joback Method
cpg	399.17	J/mol×K	585.07	Joback Method
cpg	413.59	J/mol×K	618.51	Joback Method
cpg	427.13	J/mol×K	651.95	Joback Method
cpg	439.91	J/mol×K	685.39	Joback Method
cpg	452.03	J/mol×K	718.83	Joback Method
cpg	463.60	J/mol×K	752.27	Joback Method

Sources

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R613439&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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

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