cis,trans,trans-2-Ethyl-1,4-dimethylcyclopentane

Other names: 1-trans-4-dimethyl-trans-2-ethylcyclopentane
cis,trans.trans-2-Ethyl-1,4-dimethylcyclohexane
Inchi: InChI=1S/C9H18/c1-4-9-6-7(2)5-8(9)3/h7-9H,4-6H2,1-3H3/t7-,8-,9-/m0/s1
InchiKey: VMCXXGFUCWAIIN-CIUDSAMLSA-N
Formula: C9H18
SMILES: CCC1CC(C)CC1C
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	46.03	kJ/mol	Joback Method
hf	-209.29	kJ/mol	Joback Method
hfus	15.14	kJ/mol	Joback Method
hvap	35.27	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	844.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	839.70		NIST Webbook
rinpol	843.60		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	842.00		NIST Webbook
tb	411.26	K	Joback Method
tc	601.43	K	Joback Method
tf	193.61	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	255.59	J/mol×K	411.26	Joback Method
cpg	273.61	J/mol×K	442.96	Joback Method
cpg	290.88	J/mol×K	474.65	Joback Method
cpg	307.41	J/mol×K	506.35	Joback Method
cpg	323.20	J/mol×K	538.04	Joback Method
cpg	338.29	J/mol×K	569.74	Joback Method
cpg	352.67	J/mol×K	601.43	Joback Method
dvisc	0.0013588	Pa×s	193.61	Joback Method
dvisc	0.0008515	Pa×s	229.89	Joback Method
dvisc	0.0006061	Pa×s	266.16	Joback Method
dvisc	0.0004681	Pa×s	302.44	Joback Method
dvisc	0.0003821	Pa×s	338.71	Joback Method
dvisc	0.0003244	Pa×s	374.99	Joback Method
dvisc	0.0002834	Pa×s	411.26	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R93024&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume