cis,trans,trans-3-Ethyl-1,2-dimethylcyclopentane

Inchi: InChI=1S/C9H18/c1-4-9-6-5-7(2)8(9)3/h7-9H,4-6H2,1-3H3/t7-,8+,9-/m0/s1
InchiKey: UMUGNPFWQJAOJI-YIZRAAEISA-N
Formula: C9H18
SMILES: CCC1CCC(C)C1C
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	884.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	874.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R96490&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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