

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

Other names:	1-cis-2-dimethyl-trans-3-ethylcyclopentane
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	878.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	880.50		NIST Webbook
rinpol	875.70		NIST Webbook
tb	411.26	K	Joback Method
tc	601.43	K	Joback Method
tf	193.61	K	Joback Method
vc	0.478	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.59	J/molxK	411.26	Joback Method
cpg	273.61	J/molxK	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	Paxs	193.61	Joback Method
dvisc	0.0008515	Paxs	229.89	Joback Method
dvisc	0.0006061	Paxs	266.16	Joback Method
dvisc	0.0004681	Paxs	302.44	Joback Method
dvisc	0.0003821	Paxs	338.71	Joback Method
dvisc	0.0003244	Paxs	374.99	Joback Method
dvisc	0.0002834	Paxs	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=R96440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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