1-trans-2-dimethyl-cis-4-ethylcyclopentane

Inchi: InChI=1S/C9H18/c1-4-9-5-7(2)8(3)6-9/h7-9H,4-6H2,1-3H3/t7-,8-/m0/s1
InchiKey: QKXQNQVXTYSGKS-YUMQZZPRSA-N
Formula: C9H18
SMILES: CCC1CC(C)C(C)C1
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	848.10		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.90		NIST Webbook
rinpol	844.20		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R164640&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

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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