

1-trans-3-dimethyl-1-ethylcyclopentane

Inchi:	InChI=1S/C9H18/c1-4-9(3)6-5-8(2)7-9/h8H,4-7H2,1-3H3/t8-,9+/m1/s1
InchiKey:	OAWOMHRJVJMDLZ-BDAKNGLRSA-N
Formula:	C9H18
SMILES:	CCC1(C)CCC(C)C1
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
gf	48.25	kJ/mol	Joback Method
hf	-173.71	kJ/mol	Joback Method
hfus	7.77	kJ/mol	Joback Method
hvap	34.42	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinsol	843.20		NIST Webbook
tb	416.17	K	Joback Method
tc	615.40	K	Joback Method
tf	221.75	K	Joback Method
vc	0.477	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.68	J/mol×K	416.17	Joback Method
cpg	275.18	J/mol×K	449.38	Joback Method
cpg	292.53	J/mol×K	482.58	Joback Method
cpg	308.81	J/mol×K	515.79	Joback Method
cpg	324.12	J/mol×K	548.99	Joback Method
cpg	338.53	J/mol×K	582.20	Joback Method
cpg	352.15	J/mol×K	615.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R164739&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	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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