1-trans-2-methylisopropylcyclopentane

Inchi: InChI=1S/C9H18/c1-7(2)9-6-4-5-8(9)3/h7-9H,4-6H2,1-3H3/t8-,9+/m0/s1
InchiKey: CGWXYEIWDQDFIU-DTWKUNHWSA-N
Formula: C9H18
SMILES: CC(C)C1CCCC1C
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	51.30	kJ/mol	Joback Method
hf	-194.23	kJ/mol	Joback Method
hfus	10.55	kJ/mol	Joback Method
hvap	35.19	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	870.40		NIST Webbook
rinpol	868.90		NIST Webbook
tb	415.49	K	Joback Method
tc	610.70	K	Joback Method
tf	182.85	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.75	J/mol×K	415.49	Joback Method
cpg	274.05	J/mol×K	448.03	Joback Method
cpg	291.51	J/mol×K	480.56	Joback Method
cpg	308.15	J/mol×K	513.10	Joback Method
cpg	323.99	J/mol×K	545.63	Joback Method
cpg	339.06	J/mol×K	578.17	Joback Method
cpg	353.37	J/mol×K	610.70	Joback Method
dvisc	0.0039722	Pa×s	182.85	Joback Method

dvisc	0.0017463	Pa×s	221.62	Joback Method
dvisc	0.0009806	Pa×s	260.40	Joback Method
dvisc	0.0006395	Pa×s	299.17	Joback Method
dvisc	0.0004600	Pa×s	337.94	Joback Method
dvisc	0.0003541	Pa×s	376.72	Joback Method
dvisc	0.0002863	Pa×s	415.49	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=R164675&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