trans-1-methyl-2-propylcyclopentane

Other names: Cyclopentane, 1-methyl-2-propyl-, trans-
1-trans-2-methylpropylcyclopentane
1-Methyl-2-propylcyclopentane, trans
Inchi: InChI=1S/C9H18/c1-3-5-9-7-4-6-8(9)2/h8-9H,3-7H2,1-2H3/t8-,9-/m1/s1
InchiKey: ADQJFBQXLAAVQA-IUCAKERBSA-N
Formula: C9H18
SMILES: CCC[C@@H]1CCC[C@H]1C
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
af	0.2780		Cheméo Relay (1.0)
gf	53.74	kJ/mol	Joback Method
hf	-165.58	kJ/mol	Cheméo Relay (1.0)
hfus	14.07	kJ/mol	Joback Method
hvap	42.29	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-4.92		Cheméo Relay (1.0)
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	913.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	886.60		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	881.40		NIST Webbook
rinpol	885.10		NIST Webbook
tb	413.91	K	Cheméo Relay (1.0)
tc	633.12	K	Cheméo Relay (1.0)
tf	150.00 ± 2.00	K	NIST Webbook
vc	0.485	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.81	J/mol×K	415.93	Joback Method
cpg	350.98	J/mol×K	606.59	Joback Method
cpg	336.97	J/mol×K	574.81	Joback Method
cpg	322.25	J/mol×K	543.03	Joback Method
cpg	306.79	J/mol×K	511.26	Joback Method
cpg	290.58	J/mol×K	479.48	Joback Method
cpg	273.59	J/mol×K	447.71	Joback Method
dvisc	0.0006014	Pa×s	306.89	Joback Method
dvisc	0.0002982	Pa×s	415.93	Joback Method
dvisc	0.0003603	Pa×s	379.58	Joback Method
dvisc	0.0004530	Pa×s	343.24	Joback Method
dvisc	0.0026275	Pa×s	197.85	Joback Method
dvisc	0.0008615	Pa×s	270.54	Joback Method
dvisc	0.0013798	Pa×s	234.20	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C932445&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie:	Ionization energy
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