1,2,3,4,5-pentamethylcyclohexane

Other names: 1,2,3,4,5-pentamethylcyclohexane
Inchi: InChI=1S/C11H22/c1-7-6-8(2)10(4)11(5)9(7)3/h7-11H,6H2,1-5H3
InchiKey: OPJUNOQIDNTDPN-UHFFFAOYSA-N
Formula: C11H22
SMILES: CC1CC(C)C(C)C(C)C1C
Mol. weight [g/mol]: 154.29
CAS: 1839-64-1

Physical Properties

Property code	Value	Unit	Source
hfus	20.36	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Cheméo Relay (1.0)
ie	9.08	eV	Cheméo Relay (1.0)
logp	3.571		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
tb	467.55 ± 1.50	K	NIST Webbook
tb	463.00 ± 6.00	K	NIST Webbook
tf	235.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.24	J/mol×K	451.95	Joback Method
cpg	366.80	J/mol×K	484.15	Joback Method
cpg	387.51	J/mol×K	516.35	Joback Method
cpg	407.38	J/mol×K	548.55	Joback Method
cpg	426.40	J/mol×K	580.76	Joback Method
cpg	444.58	J/mol×K	612.96	Joback Method
cpg	461.92	J/mol×K	645.16	Joback Method
dvisc	0.0009574	Pa×s	204.15	Joback Method
dvisc	0.0006447	Pa×s	245.45	Joback Method
dvisc	0.0004865	Pa×s	286.75	Joback Method
dvisc	0.0003941	Pa×s	328.05	Joback Method
dvisc	0.0003347	Pa×s	369.35	Joback Method

dvisc	0.0002937	Pa×s	410.65	Joback Method
dvisc	0.0002640	Pa×s	451.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1839641&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point