Pentane, 2-chloro-3-methyl

Inchi: InChI=1S/C6H13Cl/c1-4-5(2)6(3)7/h5-6H,4H2,1-3H3
InchiKey: JPFZKJQZKBEPGQ-UHFFFAOYSA-N
Formula: C6H13Cl
SMILES: CCC(C)C(C)Cl
Mol. weight [g/mol]: 120.62
CAS: 24319-09-3

Physical Properties

Property code	Value	Unit	Source
gf	-17.17	kJ/mol	Joback Method
hf	-193.47	kJ/mol	Joback Method
hfus	8.45	kJ/mol	Joback Method
hvap	32.56	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.660		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	787.00		NIST Webbook
rinpol	787.00		NIST Webbook
tb	373.23	K	Joback Method
tc	553.82	K	Joback Method
tf	157.30	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.75	J/mol×K	373.23	Joback Method
cpg	196.81	J/mol×K	403.33	Joback Method
cpg	207.42	J/mol×K	433.43	Joback Method
cpg	217.60	J/mol×K	463.52	Joback Method
cpg	227.35	J/mol×K	493.62	Joback Method
cpg	236.69	J/mol×K	523.72	Joback Method
cpg	245.63	J/mol×K	553.82	Joback Method

dvisc	0.0170744	Pa×s	157.30	Joback Method
dvisc	0.0045226	Pa×s	193.29	Joback Method
dvisc	0.0018178	Pa×s	229.28	Joback Method
dvisc	0.0009357	Pa×s	265.26	Joback Method
dvisc	0.0005644	Pa×s	301.25	Joback Method
dvisc	0.0003793	Pa×s	337.24	Joback Method
dvisc	0.0002752	Pa×s	373.23	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=C24319093&Units=SI

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