3-[1-METHYLETHYL]-1-CYCLOHEXENE

Other names: 3-isopropylcyclohexene
3-Isopropylcyclohexene-1
Inchi: InChI=1S/C9H16/c1-8(2)9-6-4-3-5-7-9/h4,6,8-9H,3,5,7H2,1-2H3
InchiKey: HKZXDFQIKRFLMW-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC(C)C1C=CCCC1
Mol. weight [g/mol]: 124.23

Physical Properties

Property code	Value	Unit	Source
hfus	8.60	kJ/mol	Joback Method
ie	8.86	eV	Cheméo Relay (1.0)
logp	2.999		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
rinpol	926.50		NIST Webbook
rinpol	926.10		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	915.90		NIST Webbook
rinpol	921.00		NIST Webbook
ripol	1081.00		NIST Webbook
ripol	1062.80		NIST Webbook
ripol	1043.80		NIST Webbook
ripol	1053.90		NIST Webbook
ripol	1049.00		NIST Webbook
ripol	1062.80		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1093.00		NIST Webbook
ripol	1081.00		NIST Webbook
ripol	1049.00		NIST Webbook
tb	421.22	K	Cheméo Relay (1.0)
tf	170.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.39	J/mol×K	423.59	Joback Method
cpg	259.26	J/mol×K	457.90	Joback Method
cpg	276.23	J/mol×K	492.21	Joback Method
cpg	292.30	J/mol×K	526.53	Joback Method
cpg	307.52	J/mol×K	560.84	Joback Method
cpg	321.90	J/mol×K	595.15	Joback Method
cpg	335.48	J/mol×K	629.46	Joback Method
dvisc	0.0107110	Pa×s	184.33	Joback Method
dvisc	0.0032873	Pa×s	224.21	Joback Method
dvisc	0.0014413	Pa×s	264.08	Joback Method
dvisc	0.0007846	Pa×s	303.96	Joback Method
dvisc	0.0004918	Pa×s	343.84	Joback Method
dvisc	0.0003397	Pa×s	383.71	Joback Method
dvisc	0.0002516	Pa×s	423.59	Joback Method

Sources

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
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=C3983082&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point