3-Isopropylcyclopentene

Other names: Cyclopentene,3-(1-methylethyl)-
3-[1-Methylethyl]-1-cyclopentene
3-Isopropylcyclopentene-1
Inchi: InChI=1S/C8H14/c1-7(2)8-5-3-4-6-8/h3,5,7-8H,4,6H2,1-2H3
InchiKey: WGGDPEMWUJIPOF-UHFFFAOYSA-N
Formula: C8H14
SMILES: CC(C)C1C=CCC1
Mol. weight [g/mol]: 110.20
CAS: 4276-45-3

Physical Properties

Property code	Value	Unit	Source
gf	80.55	kJ/mol	Joback Method
hf	-95.47	kJ/mol	Joback Method
hfus	8.11	kJ/mol	Joback Method
hvap	33.56	kJ/mol	Joback Method
ie	8.85 ± 0.05	eV	NIST Webbook
ie	8.81 ± 0.02	eV	NIST Webbook
log10ws	-2.44		Crippen Method
logp	2.609		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	789.70		NIST Webbook
rinpol	794.90		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	795.00		NIST Webbook

rinpol	789.70		NIST Webbook
rinpol	795.00		NIST Webbook
ripol	928.30		NIST Webbook
ripol	913.10		NIST Webbook
ripol	928.00		NIST Webbook
ripol	913.00		NIST Webbook
ripol	921.00		NIST Webbook
ripol	928.00		NIST Webbook
ripol	928.30		NIST Webbook
ripol	913.10		NIST Webbook
ripol	921.10		NIST Webbook
ripol	921.10		NIST Webbook
tb	394.00 ± 3.00	K	NIST Webbook
tb	400.80 ± 1.50	K	NIST Webbook
tb	394.40 ± 1.00	K	NIST Webbook
tb	394.40 ± 0.40	K	NIST Webbook
tc	595.92	K	Joback Method
tf	176.58	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.14	J/mol×K	396.44	Joback Method
cpg	216.87	J/mol×K	429.69	Joback Method
cpg	231.80	J/mol×K	462.93	Joback Method
cpg	245.95	J/mol×K	496.18	Joback Method
cpg	259.35	J/mol×K	529.43	Joback Method
cpg	272.03	J/mol×K	562.68	Joback Method
cpg	284.01	J/mol×K	595.92	Joback Method
dvisc	0.0049498	Pa×s	176.58	Joback Method
dvisc	0.0020283	Pa×s	213.22	Joback Method
dvisc	0.0010797	Pa×s	249.87	Joback Method
dvisc	0.0006754	Pa×s	286.51	Joback Method
dvisc	0.0004699	Pa×s	323.15	Joback Method
dvisc	0.0003520	Pa×s	359.80	Joback Method
dvisc	0.0002781	Pa×s	396.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4276453&Units=SI
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

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume