1-Methyl-3-isoallylbenzene

Inchi: InChI=1S/C10H12/c1-3-5-10-7-4-6-9(2)8-10/h3-8H,1-2H3/b5-3+
InchiKey: UUOANSACYXAAOU-HWKANZROSA-N
Formula: C10H12
SMILES: CC=Cc1cccc(C)c1
Mol. weight [g/mol]: 132.20

Physical Properties

Property code	Value	Unit	Source
gf	216.32	kJ/mol	Joback Method
hf	92.55	kJ/mol	Joback Method
hfus	15.51	kJ/mol	Joback Method
hvap	40.75	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.028		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1102.30		NIST Webbook
tb	464.02	K	Joback Method
tc	680.34	K	Joback Method
tf	236.32	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.90	J/mol×K	464.02	Joback Method
cpg	255.19	J/mol×K	500.07	Joback Method
cpg	268.61	J/mol×K	536.13	Joback Method
cpg	281.21	J/mol×K	572.18	Joback Method
cpg	293.02	J/mol×K	608.23	Joback Method
cpg	304.09	J/mol×K	644.28	Joback Method
cpg	314.47	J/mol×K	680.34	Joback Method
dvisc	0.0022393	Pa×s	236.32	Joback Method
dvisc	0.0011023	Pa×s	274.27	Joback Method

dvisc	0.0006447	Pa×s	312.22	Joback Method
dvisc	0.0004235	Pa×s	350.17	Joback Method
dvisc	0.0003021	Pa×s	388.12	Joback Method
dvisc	0.0002288	Pa×s	426.07	Joback Method
dvisc	0.0001814	Pa×s	464.02	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=R11353&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