

3-isopropyl styrene

Other names:	1-Vinyl-3-isopropylbenzene
Inchi:	InChI=1S/C11H14/c1-4-10-6-5-7-11(8-10)9(2)3/h4-9H,1H2,2-3H3
InchiKey:	BYYLJVQCWRRFMP-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	<chem>C=Cc1cccc(C(C)C)c1</chem>
Mol. weight [g/mol]:	146.23

Physical Properties

Property code	Value	Unit	Source
gf	229.92	kJ/mol	Joback Method
hf	74.84	kJ/mol	Joback Method
hfus	13.09	kJ/mol	Joback Method
hvap	41.96	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.453		Crippen Method
mvol	137.790	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1117.40		NIST Webbook
rinpol	1117.40		NIST Webbook
tb	478.98	K	Joback Method
tc	691.48	K	Joback Method
tf	235.91	K	Joback Method
vc	0.518	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.42	J/mol×K	478.98	Joback Method
cpg	298.89	J/mol×K	514.40	Joback Method
cpg	313.48	J/mol×K	549.81	Joback Method
cpg	327.21	J/mol×K	585.23	Joback Method
cpg	340.14	J/mol×K	620.64	Joback Method
cpg	352.28	J/mol×K	656.06	Joback Method
cpg	363.69	J/mol×K	691.48	Joback Method

dvisc	0.0032866	Paxs	235.91	Joback Method
dvisc	0.0014646	Paxs	276.42	Joback Method
dvisc	0.0008025	Paxs	316.93	Joback Method
dvisc	0.0005040	Paxs	357.45	Joback Method
dvisc	0.0003479	Paxs	397.96	Joback Method
dvisc	0.0002572	Paxs	438.47	Joback Method
dvisc	0.0002001	Paxs	478.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R11406&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

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

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