o-Isopropenyltoluene

Other names:	1-Isopropenyl-2-methylbenzene
	1-Methyl-2-(1-methylethenyl)-benzene
	1-Methyl-2-iso-propenylbenzene
	Benzene, 1-methyl-2-(1-methylethenyl)-
	Styrene, o,«alpha»-dimethyl-
	Styrene, o,Â«alphaÂ»-dimethyl-
	o,«alpha»-Dimethylstyrene
	o,Â«alphaÂ»-Dimethylstyrene
	o-Cymenene
	o-Methyl-«alpha»-methylstyrene
	o-Methyl-Â«alphaÂ»-methylstyrene
Inchi:	InChI=1S/C10H12/c1-8(2)10-7-5-4-6-9(10)3/h4-7H,1H2,2-3H3
InchiKey:	OGMSGZZPTQNTIK-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	C=C(C)c1ccccc1C
Mol. weight [g/mol]:	132.20
CAS:	7399-49-7

Physical Properties

Property code	Value	Unit	Source
affp	857.80	kJ/mol	NIST Webbook
basg	828.90	kJ/mol	NIST Webbook
gf	215.39	kJ/mol	Joback Method
hf	90.97	kJ/mol	Joback Method
hfus	12.72	kJ/mol	Joback Method
hvap	40.20	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.028		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1117.00		NIST Webbook
tb	445.35 ± 1.00	K	NIST Webbook
tb	448.15 ± 3.00	K	NIST Webbook
tb	445.65 ± 2.00	K	NIST Webbook
tb	441.65 ± 2.00	K	NIST Webbook

tb	442.00 ± 3.00	K	NIST Webbook
tc	671.23	K	Joback Method
tf	225.68	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.50	J/mol×K	456.42	Joback Method
cpg	254.75	J/mol×K	492.22	Joback Method
cpg	268.18	J/mol×K	528.02	Joback Method
cpg	280.82	J/mol×K	563.82	Joback Method
cpg	292.71	J/mol×K	599.62	Joback Method
cpg	303.88	J/mol×K	635.42	Joback Method
cpg	314.37	J/mol×K	671.23	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7399497&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
KDB: https://www.cheric.org/files/research/kdb/mol/mol737.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
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