Benzene, 1-(1-methylethenyl)-4-(1-methylethyl)-

Other names: 1-Isopropenyl-4-isopropylbenzene
2-(4-Isopropylphenyl)-1-propene
2-(p-Isopropylphenyl)propene
4-Isopropyl-«alpha»-methylstyrene
4-Isopropyl-Â«alphaÂ»-methylstyrene
4-Isopropylidene-cumene
Styrene, p-isopropyl-«alpha»-methyl-
Styrene, p-isopropyl-Â«alphaÂ»-methyl-
p-Isopropenylisopropylbenzene
p-Isopropyl-«alpha»-methylstyrene
p-Isopropyl-Â«alphaÂ»-methylstyrene
p-Isopropylisopropenylbenzene
«alpha»-Methyl-4-isopropylstyrene
Â«alphaÂ»-Methyl-4-isopropylstyrene

Inchi: InChI=1S/C12H16/c1-9(2)11-5-7-12(8-6-11)10(3)4/h5-8,10H,1H2,2-4H3

InchiKey: XMCNZCCURGYSDQ-UHFFFAOYSA-N

Formula: C12H16

SMILES: C=C(C)c1ccc(C(C)C)cc1

Mol. weight [g/mol]: 160.26

CAS: 2388-14-9

Physical Properties

Property code	Value	Unit	Source
gf	229.79	kJ/mol	Joback Method
hf	44.41	kJ/mol	Joback Method
hfus	14.37	kJ/mol	Joback Method
hvap	44.27	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.843		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	501.74	K	Joback Method
tc	715.12	K	Joback Method
tf	233.22	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.95	J/mol×K	679.56	Joback Method
cpg	327.95	J/mol×K	501.74	Joback Method
cpg	344.58	J/mol×K	537.30	Joback Method
cpg	360.26	J/mol×K	572.87	Joback Method
cpg	375.02	J/mol×K	608.43	Joback Method
cpg	388.90	J/mol×K	644.00	Joback Method
cpg	414.20	J/mol×K	715.12	Joback Method
hvapt	50.90	kJ/mol	441.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44494e+01
Coeff. B	-4.08840e+03
Coeff. C	-7.84680e+01
Temperature range (K), min.	367.16
Temperature range (K), max.	525.88

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2388149&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume