

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

Other names:	p-iodocumene
Inchi:	InChI=1S/C9H11I/c1-7(2)8-3-5-9(10)6-4-8/h3-7H,1-2H3
InchiKey:	PQJOSEVTIKYWHLH-UHFFFAOYSA-N
Formula:	C9H11I
SMILES:	CC(C)c1ccc(I)cc1
Mol. weight [g/mol]:	246.09
CAS:	17356-09-1

Physical Properties

Property code	Value	Unit	Source
gf	183.36	kJ/mol	Joback Method
hf	67.56	kJ/mol	Joback Method
hfus	13.60	kJ/mol	Joback Method
hvap	47.55	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.415		Crippen Method
mcvol	139.730	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	529.68	K	Joback Method
tc	778.79	K	Joback Method
tf	273.19	K	Joback Method
vc	0.513	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.33	J/molxK	529.68	Joback Method
cpg	279.71	J/molxK	571.20	Joback Method
cpg	292.13	J/molxK	612.72	Joback Method
cpg	303.63	J/molxK	654.24	Joback Method
cpg	314.28	J/molxK	695.76	Joback Method
cpg	324.14	J/molxK	737.28	Joback Method
cpg	333.25	J/molxK	778.79	Joback Method
dvisc	0.0039156	Paxs	273.19	Joback Method

dvisc	0.0018323	Paxs	315.94	Joback Method
dvisc	0.0010275	Paxs	358.69	Joback Method
dvisc	0.0006518	Paxs	401.44	Joback Method
dvisc	0.0004513	Paxs	444.18	Joback Method
dvisc	0.0003333	Paxs	486.93	Joback Method
dvisc	0.0002585	Paxs	529.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17356091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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