

Benzenemethanol, 3-iodo-

Other names:	Benzyl alcohol, m-iodo- m-Iodobenzyl alcohol 3-Iodobenzyl alcohol (3-Iodophenyl)methanol
Inchi:	InChI=1S/C7H7IO/c8-7-3-1-2-6(4-7)5-9/h1-4,9H,5H2
InchiKey:	QGCCNWSXJHGUNL-UHFFFAOYSA-N
Formula:	C7H7IO
SMILES:	OCc1cccc(I)c1
Mol. weight [g/mol]:	234.03
CAS:	57455-06-8

Physical Properties

Property code	Value	Unit	Source
gf	32.14	kJ/mol	Joback Method
hf	-38.11	kJ/mol	Joback Method
hfus	16.03	kJ/mol	Joback Method
hvap	60.17	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.784		Crippen Method
mcvol	117.420	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
tb	576.54	K	Joback Method
tc	807.96	K	Joback Method
tf	326.47	K	Joback Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.33	J/molxK	576.54	Joback Method
cpg	257.60	J/molxK	769.39	Joback Method
cpg	251.41	J/molxK	730.82	Joback Method
cpg	244.73	J/molxK	692.25	Joback Method
cpg	237.52	J/molxK	653.68	Joback Method

cpg	229.73	J/molxK	615.11	Joback Method
cpg	263.35	J/molxK	807.96	Joback Method
dvisc	0.0001284	Paxs	576.54	Joback Method
dvisc	0.0001932	Paxs	534.86	Joback Method
dvisc	0.0003117	Paxs	493.18	Joback Method
dvisc	0.0005493	Paxs	451.50	Joback Method
dvisc	0.0010861	Paxs	409.83	Joback Method
dvisc	0.0025061	Paxs	368.15	Joback Method
dvisc	0.0071586	Paxs	326.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	525.20	K	94.80	NIST Webbook

Sources

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=C57455068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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