

Benzene, (3-iodopropyl)-

Other names:	1-Iodo-3-phenylpropane 3-Phenylpropyl iodide (3-Iodopropyl)benzene
Inchi:	InChI=1S/C9H11I/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2
InchiKey:	RGCKJSPKMTWLLX-UHFFFAOYSA-N
Formula:	C9H11I
SMILES:	ICCCc1ccccc1
Mol. weight [g/mol]:	246.09
CAS:	4119-41-9

Physical Properties

Property code	Value	Unit	Source
gf	195.43	kJ/mol	Joback Method
hf	84.31	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	47.28	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.054		Crippen Method
mcvol	139.730	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	525.14	K	Joback Method
tc	767.16	K	Joback Method
tf	275.67	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.38	J/mol×K	525.14	Joback Method
cpg	279.78	J/mol×K	565.48	Joback Method
cpg	292.18	J/mol×K	605.81	Joback Method
cpg	303.65	J/mol×K	646.15	Joback Method
cpg	314.26	J/mol×K	686.48	Joback Method
cpg	324.07	J/mol×K	726.82	Joback Method

cpg	333.14	J/mol×K	767.16	Joback Method
dvisc	0.0040683	Pa×s	275.67	Joback Method
dvisc	0.0019501	Pa×s	317.25	Joback Method
dvisc	0.0011084	Pa×s	358.83	Joback Method
dvisc	0.0007085	Pa×s	400.40	Joback Method
dvisc	0.0004926	Pa×s	441.98	Joback Method
dvisc	0.0003646	Pa×s	483.56	Joback Method
dvisc	0.0002830	Pa×s	525.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4119419&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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