

1-Propanol, 3-iodo-

Other names:	3-Iodo-1-propanol 3-iodopropanol
Inchi:	InChI=1S/C3H7IO/c4-2-1-3-5/h5H,1-3H2
InchiKey:	CQVWOJSAGPFDQL-UHFFFAOYSA-N
Formula:	C3H7IO
SMILES:	OCCCI
Mol. weight [g/mol]:	185.99
CAS:	627-32-7

Physical Properties

Property code	Value	Unit	Source
gf	-104.32	kJ/mol	Joback Method
hf	-180.61	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	48.32	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	0.804		Crippen Method
mvol	84.820	ml/mol	McGowan Method
pc	4849.43	kPa	Joback Method
tb	453.36	K	Joback Method
tc	649.65	K	Joback Method
tf	242.45	K	Joback Method
vc	0.310	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.45	J/molxK	453.36	Joback Method
cpg	162.16	J/molxK	616.94	Joback Method
cpg	157.57	J/molxK	584.22	Joback Method
cpg	152.72	J/molxK	551.51	Joback Method
cpg	147.59	J/molxK	518.79	Joback Method
cpg	142.18	J/molxK	486.08	Joback Method
cpg	166.51	J/molxK	649.65	Joback Method

dvisc	0.0003459	Paxs	453.36	Joback Method
dvisc	0.0005672	Paxs	418.21	Joback Method
dvisc	0.0010185	Paxs	383.06	Joback Method
dvisc	0.0020586	Paxs	347.90	Joback Method
dvisc	0.0048740	Paxs	312.75	Joback Method
dvisc	0.0143550	Paxs	277.60	Joback Method
dvisc	0.0578296	Paxs	242.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	0.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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