3-Iodopropanol

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

Physical Properties

Property code	Value	Unit	Source
hf	-194.06	kJ/mol	Cheméo Relay (1.0)
hfus	12.02	kJ/mol	Joback Method
hvap	66.87	kJ/mol	Cheméo Relay (1.0)
ie	9.47	eV	Cheméo Relay (1.0)
logp	0.804		Crippen Method
mcvol	84.820	ml/mol	McGowan Method
pc	4849.43	kPa	Joback Method
tb	481.83	K	Cheméo Relay (1.0)
tc	753.80	K	Cheméo Relay (1.0)
tf	232.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.45	J/mol×K	453.36	Joback Method
cpg	142.18	J/mol×K	486.08	Joback Method
cpg	147.59	J/mol×K	518.79	Joback Method
cpg	152.72	J/mol×K	551.51	Joback Method
cpg	157.57	J/mol×K	584.22	Joback Method
cpg	162.16	J/mol×K	616.94	Joback Method
cpg	166.51	J/mol×K	649.65	Joback Method
dvisc	0.0578296	Pa×s	242.45	Joback Method
dvisc	0.0143550	Pa×s	277.60	Joback Method
dvisc	0.0048740	Pa×s	312.75	Joback Method

dvisc	0.0020586	Pa×s	347.90	Joback Method
dvisc	0.0010185	Pa×s	383.06	Joback Method
dvisc	0.0005672	Pa×s	418.21	Joback Method
dvisc	0.0003459	Pa×s	453.36	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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C627327&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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