

3-Iodo-1,2-propanediol

Inchi:	InChI=1S/C3H7IO2/c4-1-3(6)2-5/h3,5-6H,1-2H2
InchiKey:	GLJRUXJFSCIQFV-UHFFFAOYSA-N
Formula:	C3H7IO2
SMILES:	OCC(O)CI
Mol. weight [g/mol]:	201.99
CAS:	554-10-9

Physical Properties

Property code	Value	Unit	Source
hf	-375.45	kJ/mol	Cheméo Relay (1.0)
hfus	12.58	kJ/mol	Joback Method
hvap	86.98	kJ/mol	Cheméo Relay (1.0)
log10ws	0.29		Cheméo Relay (1.0)
logp	-0.225		Crippen Method
mcvol	90.690	ml/mol	McGowan Method
pc	5602.57	kPa	Joback Method
tb	547.64	K	Cheméo Relay (1.0)
tc	838.24	K	Cheméo Relay (1.0)
tf	321.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.309	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	2.07520e+01
Coeff. B	4.01700e-01
Coeff. C	-2.84800e-04
Coeff. D	8.35000e-08
Coeff. E	0.00000e+00

Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-1.74428e+01
Coeff. B	4.42534e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from T_f to $0.7 \cdot T_c$.
Temperature range (K), min.	321.65
Temperature range (K), max.	514.36

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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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