Acetic acid, iodo-, ethyl ester

Other names:	Ethyl iodoacetate
	Ethyl monoiodoacetate
	Iodoacetic acid, ethyl ester
	S 9
Inchi:	InChI=1S/C4H7IO2/c1-2-7-4(6)3-5/h2-3H2,1H3
InchiKey:	MFFXVVHUKRKXCI-UHFFFAOYSA-N
Formula:	C4H7IO2
SMILES:	CCOC(=O)CI
Mol. weight [g/mol]:	214.00
CAS:	623-48-3

Physical Properties

Property code	Value	Unit	Source
af	0.3783		Cheméo Relay (1.0)
gf	-193.00	kJ/mol	Joback Method
hf	-351.19	kJ/mol	Cheméo Relay (1.0)
hfus	13.31	kJ/mol	Joback Method
hvap	48.41	kJ/mol	Cheméo Relay (1.0)
ie	9.68	eV	Cheméo Relay (1.0)
log10ws	-1.37		Cheméo Relay (1.0)
logp	0.984		Crippen Method
mcvol	100.480	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	960.50		NIST Webbook
tb	452.20	K	NIST Webbook
tc	674.44	K	Cheméo Relay (1.0)
tf	282.28	K	Cheméo Relay (1.0)
vc	0.354	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.84	J/mol×K	460.35	Joback Method
cpg	174.08	J/mol×K	496.35	Joback Method

cpg	180.99	J/mol×K	532.35	Joback Method
cpg	187.57	J/mol×K	568.35	Joback Method
cpg	193.82	J/mol×K	604.35	Joback Method
cpg	199.76	J/mol×K	640.34	Joback Method
cpg	205.39	J/mol×K	676.34	Joback Method
dvisc	0.0037331	Pa×s	265.06	Joback Method
dvisc	0.0020858	Pa×s	297.61	Joback Method
dvisc	0.0013071	Pa×s	330.16	Joback Method
dvisc	0.0008908	Pa×s	362.71	Joback Method
dvisc	0.0006466	Pa×s	395.25	Joback Method
dvisc	0.0004929	Pa×s	427.80	Joback Method
dvisc	0.0003904	Pa×s	460.35	Joback Method
hvapt	52.10	kJ/mol	331.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.20	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.84853e+01
Coeff. B	-6.26994e+03
Temperature range (K), min.	344.55
Temperature range (K), max.	475.94

Sources

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):

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623483&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume