

«beta»-Iodoethyl acetate

Other names:	Acetic acid, 2-iodoethyl ester
Inchi:	InChI=1S/C4H7IO2/c1-4(6)7-3-2-5/h2-3H2,1H3
InchiKey:	DYHCCCWROHIOFM-UHFFFAOYSA-N
Formula:	C4H7IO2
SMILES:	CC(=O)OCCI
Mol. weight [g/mol]:	214.00
CAS:	627-10-1

Physical Properties

Property code	Value	Unit	Source
gf	-193.00	kJ/mol	Joback Method
hf	-293.82	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	0.984		Crippen Method
mcvol	100.480	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
tb	460.35	K	Joback Method
tc	676.34	K	Joback Method
tf	265.06	K	Joback Method
vc	0.371	m3/kmol	Joback Method

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

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627101&Units=SI

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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