Benzene, (2-iodoethyl)-

Other names:	(2-Iodoethyl)benzene
	2-Phenylethyl iodide
	Phenethyl iodide
	«beta»-Phenethyl iodide
	«beta»-Phenylethyl iodide
	Â«betaÂ»-Phenethyl iodide
	Â«betaÂ»-Phenylethyl iodide
Inchi:	InChI=1S/C8H9I/c9-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	KVTHPKXDLVYNCH-UHFFFAOYSA-N
Formula:	C8H9I
SMILES:	ICCc1ccccc1
Mol. weight [g/mol]:	232.06
CAS:	17376-04-4

Physical Properties

Property code	Value	Unit	Source
gf	187.01	kJ/mol	Joback Method
hf	104.95	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	45.05	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.664		Crippen Method
mcvol	125.640	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	502.26	K	Joback Method
tc	749.17	K	Joback Method
tf	264.40	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.73	J/mol×K	502.26	Joback Method
cpg	236.02	J/mol×K	543.41	Joback Method

cpg	247.35	J/mol×K	584.56	Joback Method
cpg	257.80	J/mol×K	625.71	Joback Method
cpg	267.42	J/mol×K	666.87	Joback Method
cpg	276.29	J/mol×K	708.02	Joback Method
cpg	284.45	J/mol×K	749.17	Joback Method
dvisc	0.0041644	Pa×s	264.40	Joback Method
dvisc	0.0020345	Pa×s	304.04	Joback Method
dvisc	0.0011725	Pa×s	343.69	Joback Method
dvisc	0.0007574	Pa×s	383.33	Joback Method
dvisc	0.0005310	Pa×s	422.97	Joback Method
dvisc	0.0003956	Pa×s	462.62	Joback Method
dvisc	0.0003088	Pa×s	502.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36109e+01
Coeff. B	-3.82067e+03
Coeff. C	-8.01050e+01
Temperature range (K), min.	366.87
Temperature range (K), max.	540.46

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C17376044&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume