1-Iodo-2-butene

Inchi: InChI=1S/C4H7I/c1-2-3-4-5/h2-3H,4H2,1H3/b3-2+
InchiKey: LOPHPAWGOMDGMA-NSCUHMNNSA-N
Formula: C4H7I
SMILES: CC=CCI
Mol. weight [g/mol]: 182.00
CAS: 627-24-7

Physical Properties

Property code	Value	Unit	Source
gf	121.14	kJ/mol	Joback Method
hf	68.20	kJ/mol	Joback Method
hfus	10.72	kJ/mol	Joback Method
hvap	33.83	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.998		Crippen Method
mcvol	88.740	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	388.22	K	Joback Method
tc	603.76	K	Joback Method
tf	187.82	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	121.80	J/mol×K	388.22	Joback Method
cpg	155.10	J/mol×K	567.84	Joback Method
cpg	149.35	J/mol×K	531.92	Joback Method
cpg	143.17	J/mol×K	495.99	Joback Method
cpg	136.55	J/mol×K	460.07	Joback Method
cpg	129.44	J/mol×K	424.14	Joback Method
cpg	160.48	J/mol×K	603.76	Joback Method
dvisc	0.0003355	Pa×s	388.22	Joback Method
dvisc	0.0004295	Pa×s	354.82	Joback Method

dvisc	0.0005788	Pa×s	321.42	Joback Method
dvisc	0.0008360	Pa×s	288.02	Joback Method
dvisc	0.0013295	Pa×s	254.62	Joback Method
dvisc	0.0024324	Pa×s	221.22	Joback Method
dvisc	0.0055168	Pa×s	187.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.88485e+01
Coeff. B	-4.68362e+03
Coeff. C	-5.37820e+01
Temperature range (K), min.	306.12
Temperature range (K), max.	428.70

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=C627247&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