

1-BUTENE, 4-iodo-

Inchi:	InChI=1S/C4H7I/c1-2-3-4-5/h2H,1,3-4H2
InchiKey:	VUSYNHBKPCGGCI-UHFFFAOYSA-N
Formula:	C4H7I
SMILES:	C=CCCI
Mol. weight [g/mol]:	182.00

Physical Properties

Property code	Value	Unit	Source
af	0.1947		Cheméo Relay (1.0)
gf	128.76	kJ/mol	Joback Method
hf	80.03	kJ/mol	Cheméo Relay (1.0)
hfus	9.24	kJ/mol	Joback Method
hvap	42.14	kJ/mol	Cheméo Relay (1.0)
ie	9.28	eV	Cheméo Relay (1.0)
log10ws	-2.38		Cheméo Relay (1.0)
logp	1.998		Crippen Method
mcvol	88.740	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	391.04	K	Cheméo Relay (1.0)
tc	609.08	K	Cheméo Relay (1.0)
tf	164.61	K	Cheméo Relay (1.0)
vc	0.308	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.27	J/mol×K	380.74	Joback Method
cpg	130.59	J/mol×K	415.57	Joback Method
cpg	137.46	J/mol×K	450.39	Joback Method
cpg	143.92	J/mol×K	485.22	Joback Method
cpg	149.98	J/mol×K	520.04	Joback Method
cpg	155.68	J/mol×K	554.87	Joback Method
cpg	161.03	J/mol×K	589.69	Joback Method
dvisc	0.0050531	Pa×s	191.14	Joback Method

dvisc	0.0024463	Pa×s	222.74	Joback Method
dvisc	0.0014183	Pa×s	254.34	Joback Method
dvisc	0.0009275	Pa×s	285.94	Joback Method
dvisc	0.0006601	Pa×s	317.54	Joback Method
dvisc	0.0004996	Pa×s	349.14	Joback Method
dvisc	0.0003960	Pa×s	380.74	Joback Method

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7766510&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
ie:	Ionization energy
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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