1-IODO-2-METHYLNONANE

Inchi: InChI=1S/C10H21I/c1-3-4-5-6-7-8-10(2)9-11/h10H,3-9H2,1-2H3
InchiKey: QTODEOLPXXGOBE-UHFFFAOYSA-N
Formula: C10H21I
SMILES: CCCCCCCC(C)CI
Mol. weight [g/mol]: 268.18
CAS: ---

Physical Properties

Property code	Value	Unit	Source
af	0.4821		Cheméo Relay (1.0)
gf	89.00	kJ/mol	Joback Method
hf	-203.80	kJ/mol	Cheméo Relay (1.0)
hfus	22.54	kJ/mol	Joback Method
hvap	62.44	kJ/mol	Cheméo Relay (1.0)
ie	8.85	eV	Cheméo Relay (1.0)
log10ws	-6.06		Cheméo Relay (1.0)
logp	4.418		Crippen Method
mcvol	177.580	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
tb	515.86	K	Cheméo Relay (1.0)
tc	712.84	K	Cheméo Relay (1.0)
tf	228.92	K	Cheméo Relay (1.0)
vc	0.645	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.75	J/mol×K	520.90	Joback Method
cpg	462.88	J/mol×K	715.99	Joback Method
cpg	450.89	J/mol×K	683.47	Joback Method
cpg	438.27	J/mol×K	650.96	Joback Method
cpg	424.97	J/mol×K	618.44	Joback Method
cpg	410.97	J/mol×K	585.93	Joback Method
cpg	396.24	J/mol×K	553.41	Joback Method

dvisc	0.0007579	Pa×s	383.21	Joback Method
dvisc	0.0002436	Pa×s	520.90	Joback Method
dvisc	0.0003306	Pa×s	475.00	Joback Method
dvisc	0.0004788	Pa×s	429.11	Joback Method
dvisc	0.0084201	Pa×s	245.52	Joback Method
dvisc	0.0013594	Pa×s	337.31	Joback Method
dvisc	0.0029306	Pa×s	291.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53486e+01
Coeff. B	-4.64633e+03
Coeff. C	-8.74200e+01
Temperature range (K), min.	395.92
Temperature range (K), max.	550.33

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U101479&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume