2-Iodomesitylene

Other names:	2,4,6-trimethyliodobenzene
	Benzene, 2-iodo-1,3,5-trimethyl-
	Iodo-2,4,6-trimethylbenzene
Inchi:	InChI=1S/C9H11I/c1-6-4-7(2)9(10)8(3)5-6/h4-5H,1-3H3
InchiKey:	GTPNXFKONRIHRW-UHFFFAOYSA-N
Formula:	C9H11I
SMILES:	Cc1cc(C)c(I)c(C)c1
Mol. weight [g/mol]:	246.09
CAS:	4028-63-1

Physical Properties

Property code	Value	Unit	Source
af	0.3693		Cheméo Relay (1.0)
gf	166.54	kJ/mol	Joback Method
hf	82.95	kJ/mol	Cheméo Relay (1.0)
hfus	16.35	kJ/mol	Joback Method
hvap	58.29	kJ/mol	Cheméo Relay (1.0)
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-4.86		Cheméo Relay (1.0)
logp	3.216		Crippen Method
mcvol	139.730	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	521.11	K	Cheméo Relay (1.0)
tc	749.12	K	Cheméo Relay (1.0)
tf	299.94	K	Cheméo Relay (1.0)
vc	0.494	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.88	J/mol×K	540.08	Joback Method
cpg	277.13	J/mol×K	581.02	Joback Method
cpg	288.62	J/mol×K	621.97	Joback Method
cpg	299.39	J/mol×K	662.91	Joback Method

cpg	309.47	J/mol×K	703.85	Joback Method
cpg	318.90	J/mol×K	744.80	Joback Method
cpg	327.71	J/mol×K	785.74	Joback Method
dvisc	0.0016845	Pa×s	313.23	Joback Method
dvisc	0.0010434	Pa×s	351.04	Joback Method
dvisc	0.0007094	Pa×s	388.85	Joback Method
dvisc	0.0005165	Pa×s	426.65	Joback Method
dvisc	0.0003959	Pa×s	464.46	Joback Method
dvisc	0.0003159	Pa×s	502.27	Joback Method
dvisc	0.0002602	Pa×s	540.08	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38029e+01
Coeff. B	-4.01797e+03
Coeff. C	-8.57100e+01
Temperature range (K), min.	383.00
Temperature range (K), max.	558.89

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4028631&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

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