Phenetole, o-iodo-

Other names: Benzene, 1-ethoxy-2-iodo-
Inchi: InChI=1S/C8H9IO/c1-2-10-8-6-4-3-5-7(8)9/h3-6H,2H2,1H3
InchiKey: JUJREUXKABNEFA-UHFFFAOYSA-N
Formula: C8H9IO
SMILES: CCOc1ccccc1I
Mol. weight [g/mol]: 248.06
CAS: 614-73-3

Physical Properties

Property code	Value	Unit	Source
gf	72.38	kJ/mol	Joback Method
hf	-38.74	kJ/mol	Joback Method
hfus	15.72	kJ/mol	Joback Method
hvap	48.12	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.690		Crippen Method
mcvol	131.510	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	529.66	K	Joback Method
tc	774.42	K	Joback Method
tf	299.15	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.94	J/mol×K	529.66	Joback Method
cpg	256.53	J/mol×K	570.45	Joback Method
cpg	267.35	J/mol×K	611.25	Joback Method
cpg	277.46	J/mol×K	652.04	Joback Method
cpg	286.86	J/mol×K	692.83	Joback Method
cpg	295.59	J/mol×K	733.62	Joback Method
cpg	303.69	J/mol×K	774.42	Joback Method
dvisc	0.0022252	Pa×s	299.15	Joback Method

dvisc	0.0012464	Pa×s	337.57	Joback Method
dvisc	0.0007860	Pa×s	375.99	Joback Method
dvisc	0.0005398	Pa×s	414.40	Joback Method
dvisc	0.0003952	Pa×s	452.82	Joback Method
dvisc	0.0003038	Pa×s	491.24	Joback Method
dvisc	0.0002426	Pa×s	529.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	518.20	K	98.10	NIST Webbook
tbrp	399.20	K	2.40	NIST Webbook

Sources

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=C614733&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume