

3-Iodo-4-methoxytoluene

Inchi:	InChI=1S/C8H9IO/c1-6-3-4-8(10-2)7(9)5-6/h3-5H,1-2H3
InchiKey:	OASGOCIPNQWCLR-UHFFFAOYSA-N
Formula:	C8H9IO
SMILES:	COc1ccc(C)cc1I
Mol. weight [g/mol]:	248.06
CAS:	50597-88-1

Physical Properties

Property code	Value	Unit	Source
gf	62.75	kJ/mol	Joback Method
hf	-50.21	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.608		Crippen Method
mcvol	131.510	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	534.64	K	Joback Method
tc	780.62	K	Joback Method
tf	311.67	K	Joback Method
vc	0.481	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.26	J/molxK	534.64	Joback Method
cpg	293.73	J/molxK	739.62	Joback Method
cpg	285.12	J/molxK	698.63	Joback Method
cpg	275.88	J/molxK	657.63	Joback Method
cpg	266.00	J/molxK	616.63	Joback Method
cpg	255.47	J/molxK	575.64	Joback Method
cpg	301.74	J/molxK	780.62	Joback Method
dvisc	0.0002357	Paxs	534.64	Joback Method
dvisc	0.0002896	Paxs	497.48	Joback Method

dvisc	0.0003677	Paxs	460.32	Joback Method
dvisc	0.0004869	Paxs	423.15	Joback Method
dvisc	0.0006807	Paxs	385.99	Joback Method
dvisc	0.0010218	Paxs	348.83	Joback Method
dvisc	0.0016901	Paxs	311.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50597881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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