

5-Methoxyindane

Other names:	Indane, 5-methoxy
Inchi:	InChI=1S/C10H12O/c1-11-10-6-5-8-3-2-4-9(8)7-10/h5-7H,2-4H2,1H3
InchiKey:	WPPWEFVZGFJESZ-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	COc1ccc2c(c1)CCC2
Mol. weight [g/mol]:	148.20

Physical Properties

Property code	Value	Unit	Source
gf	89.93	kJ/mol	Joback Method
hf	-75.22	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hvap	44.09	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.184		Crippen Method
mvol	123.010	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1304.00		NIST Webbook
tb	498.67	K	Joback Method
tc	721.23	K	Joback Method
tf	298.33	K	Joback Method
vc	0.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.38	J/molxK	498.67	Joback Method
cpg	330.74	J/molxK	684.13	Joback Method
cpg	319.50	J/molxK	647.04	Joback Method
cpg	307.49	J/molxK	609.95	Joback Method
cpg	294.66	J/molxK	572.86	Joback Method
cpg	280.97	J/molxK	535.76	Joback Method
cpg	341.27	J/molxK	721.23	Joback Method
dvisc	0.0003378	Paxs	498.67	Joback Method

dvisc	0.0003921	Paxs	465.28	Joback Method
dvisc	0.0004659	Paxs	431.89	Joback Method
dvisc	0.0005697	Paxs	398.50	Joback Method
dvisc	0.0007227	Paxs	365.11	Joback Method
dvisc	0.0009619	Paxs	331.72	Joback Method
dvisc	0.0013647	Paxs	298.33	Joback Method

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=U342738&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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