INDANE-4-CARBOXALDEHYDE

Other names: Indane-4-carboxaldehyde
Indane-4-carbaldehyde
Inchi: InChI=1S/C10H10O/c11-7-9-5-1-3-8-4-2-6-10(8)9/h1,3,5,7H,2,4,6H2
InchiKey: VAZZQRFSDNZKPO-UHFFFAOYSA-N
Formula: C10H10O
SMILES: O=Cc1cccc2c1CCC2
Mol. weight [g/mol]: 146.19

Physical Properties

Property code	Value	Unit	Source
af	0.4583		Cheméo Relay (1.0)
hf	-83.30	kJ/mol	Cheméo Relay (1.0)
hfus	14.27	kJ/mol	Joback Method
hvap	64.63	kJ/mol	Cheméo Relay (1.0)
ie	8.96	eV	Cheméo Relay (1.0)
log10ws	-2.71		Cheméo Relay (1.0)
logp	1.988		Crippen Method
mcvol	118.710	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1307.00		NIST Webbook
rinpol	1307.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	1991.00		NIST Webbook
tb	532.88	K	Cheméo Relay (1.0)
tc	806.23	K	Cheméo Relay (1.0)
tf	306.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.44	J/mol×K	524.91	Joback Method
cpg	274.69	J/mol×K	563.06	Joback Method
cpg	286.96	J/mol×K	601.22	Joback Method
cpg	298.33	J/mol×K	639.37	Joback Method

cpg	308.87	J/mol×K	677.52	Joback Method
cpg	318.65	J/mol×K	715.67	Joback Method
cpg	327.74	J/mol×K	753.83	Joback Method
dvisc	0.0020037	Pa×s	318.10	Joback Method
dvisc	0.0014257	Pa×s	352.57	Joback Method
dvisc	0.0010778	Pa×s	387.04	Joback Method
dvisc	0.0008530	Pa×s	421.51	Joback Method
dvisc	0.0006993	Pa×s	455.97	Joback Method
dvisc	0.0005896	Pa×s	490.44	Joback Method
dvisc	0.0005083	Pa×s	524.91	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51932708&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point