5-Aminoindan

Other names:	5-Aminohydrindene
	5-Amino indane
	1H-Inden-5-amine, 2,3-dihydro-
	indan-5-amine
Inchi:	InChI=1S/C9H11N/c10-9-5-4-7-2-1-3-8(7)6-9/h4-6H,1-3,10H2
InchiKey:	LEWZOBYWGWKNCK-UHFFFAOYSA-N
Formula:	C9H11N
SMILES:	Nc1ccc2c(c1)CCC2
Mol. weight [g/mol]:	133.19
CAS:	24425-40-9

Physical Properties

Property code	Value	Unit	Source
gf	252.96	kJ/mol	Joback Method
hf	111.43	kJ/mol	Joback Method
hfus	14.59	kJ/mol	Joback Method
hvap	50.09	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.758		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
rinpol	232.12		NIST Webbook
rinpol	231.35		NIST Webbook
tb	525.90	K	Joback Method
tc	765.83	K	Joback Method
tf	310.50 ± 0.50	K	NIST Webbook
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.08	J/mol×K	525.90	Joback Method
cpg	268.83	J/mol×K	565.89	Joback Method
cpg	281.53	J/mol×K	605.88	Joback Method

cpg	293.27	J/mol×K	645.87	Joback Method
cpg	304.13	J/mol×K	685.86	Joback Method
cpg	314.19	J/mol×K	725.85	Joback Method
cpg	323.54	J/mol×K	765.83	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	521.20	K	99.30	NIST Webbook
tbrp	521.00 ± 1.00	K	99.30	NIST Webbook
tbrp	419.50 ± 0.50	K	3.30	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24425409&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume