1H-Inden-1-amine, 2,3-dihydro-, (.+/-.)-

Inchi: InChI=1S/C9H11N/c10-9-6-5-7-3-1-2-4-8(7)9/h1-4,9H,5-6,10H2
InchiKey: XJEVHMGJSYVQBQ-UHFFFAOYSA-N
Formula: C9H11N
SMILES: NC1CCc2ccccc21
Mol. weight [g/mol]: 133.19
CAS: 61949-83-5

Physical Properties

Property code	Value	Unit	Source
gf	254.88	kJ/mol	Joback Method
hf	102.56	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.633		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	516.25	K	Joback Method
tc	754.89	K	Joback Method
tf	331.33	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.72	J/mol×K	516.25	Joback Method
cpg	271.36	J/mol×K	556.02	Joback Method
cpg	284.89	J/mol×K	595.80	Joback Method
cpg	297.39	J/mol×K	635.57	Joback Method
cpg	308.95	J/mol×K	675.34	Joback Method
cpg	319.64	J/mol×K	715.12	Joback Method
cpg	329.54	J/mol×K	754.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	493.70	K	99.60	NIST Webbook
tbrp	369.70	K	1.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C61949835&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume