

9,10-Octalin

Inchi:	InChI=1S/C10H16/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H2
InchiKey:	ZKZCHOVDCNLSKG-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	C1CCC2=C(C1)CCCC2
Mol. weight [g/mol]:	136.23

Physical Properties

Property code	Value	Unit	Source
gf	132.54	kJ/mol	Joback Method
hf	-53.25	kJ/mol	Joback Method
hfus	7.83	kJ/mol	Joback Method
hvap	40.60	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.431		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinsol	1123.00		NIST Webbook
tb	477.22	K	Joback Method
tc	704.90	K	Joback Method
tf	258.54	K	Joback Method
vc	0.466	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.16	J/mol×K	477.22	Joback Method
cpg	357.67	J/mol×K	666.95	Joback Method
cpg	343.01	J/mol×K	629.01	Joback Method
cpg	327.29	J/mol×K	591.06	Joback Method
cpg	310.45	J/mol×K	553.11	Joback Method
cpg	292.43	J/mol×K	515.17	Joback Method
cpg	371.35	J/mol×K	704.90	Joback Method
dvisc	0.0003440	Paxs	477.22	Joback Method
dvisc	0.0004363	Paxs	440.77	Joback Method

dvisc	0.0005774	Paxs	404.33	Joback Method
dvisc	0.0008080	Paxs	367.88	Joback Method
dvisc	0.0012172	Paxs	331.43	Joback Method
dvisc	0.0020292	Paxs	294.99	Joback Method
dvisc	0.0039070	Paxs	258.54	Joback Method

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=R133032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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