

Benzene, 1-cyclopropyl-3-methyl-

Inchi: InChI=1S/C10H12/c1-8-3-2-4-10(7-8)9-5-6-9/h2-4,7,9H,5-6H2,1H3
InchiKey: RXJQJOILAUBJEG-UHFFFAOYSA-N
Formula: C10H12
SMILES: Cc1cccc(C2CC2)c1
Mol. weight [g/mol]: 132.20
CAS: 19714-73-9

Physical Properties

Property code	Value	Unit	Source
affp	835.80	kJ/mol	NIST Webbook
basg	803.30	kJ/mol	NIST Webbook
gf	196.85	kJ/mol	Joback Method
hf	48.13	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	40.70	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.872		Crippen Method
mcvol	117.140	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	466.60	K	Joback Method
tc	689.90	K	Joback Method
tf	259.34	K	Joback Method
vc	0.445	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.54	J/mol×K	466.60	Joback Method
cpg	312.26	J/mol×K	652.68	Joback Method
cpg	300.22	J/mol×K	615.47	Joback Method
cpg	287.30	J/mol×K	578.25	Joback Method
cpg	273.42	J/mol×K	541.03	Joback Method
cpg	258.52	J/mol×K	503.82	Joback Method
cpg	323.47	J/mol×K	689.90	Joback Method

dvisc	0.0003992	Paxs	466.60	Joback Method
dvisc	0.0004515	Paxs	432.06	Joback Method
dvisc	0.0005217	Paxs	397.51	Joback Method
dvisc	0.0006195	Paxs	362.97	Joback Method
dvisc	0.0007629	Paxs	328.43	Joback Method
dvisc	0.0009866	Paxs	293.88	Joback Method
dvisc	0.0013663	Paxs	259.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19714739&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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