

Benzene, (1-methylpropyl)-, (S)-

Inchi:	InChI=1S/C10H14/c1-3-9(2)10-7-5-4-6-8-10/h4-9H,3H2,1-2H3/t9-/m1/s1
InchiKey:	ZJMWRROPUADPEA-SECBINFHSA-N
Formula:	C10H14
SMILES:	CCC(C)c1ccccc1
Mol. weight [g/mol]:	134.22
CAS:	5787-28-0

Physical Properties

Property code	Value	Unit	Source
gf	143.29	kJ/mol	Joback Method
hf	-18.48	kJ/mol	Joback Method
hfus	12.17	kJ/mol	Joback Method
hvap	39.74	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.200		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
tb	454.44	K	Joback Method
tc	663.87	K	Joback Method
tf	213.88	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.43	J/mol×K	454.44	Joback Method
cpg	325.87	J/mol×K	628.97	Joback Method
cpg	313.60	J/mol×K	594.06	Joback Method
cpg	300.56	J/mol×K	559.16	Joback Method
cpg	286.70	J/mol×K	524.25	Joback Method
cpg	272.00	J/mol×K	489.35	Joback Method
cpg	337.41	J/mol×K	663.87	Joback Method
dvisc	0.0002163	Pa×s	454.44	Joback Method
dvisc	0.0002868	Pa×s	414.35	Joback Method

dvisc	0.0004037	Pa×s	374.25	Joback Method
dvisc	0.0006171	Pa×s	334.16	Joback Method
dvisc	0.0010588	Pa×s	294.07	Joback Method
dvisc	0.0021545	Pa×s	253.97	Joback Method
dvisc	0.0057217	Pa×s	213.88	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	336.20	K	2.00	NIST Webbook

Sources

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=C5787280&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

vc: Critical Volume

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