

Benzene, 1-methyl-2-octyl

Inchi:	InChI=1S/C15H24/c1-3-4-5-6-7-8-12-15-13-10-9-11-14(15)2/h9-11,13H,3-8,12H2,1-2H3
InchiKey:	RJAGGBZNYDYEPE-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CCCCCCCCc1ccccc1C
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	178.20	kJ/mol	Joback Method
hf	-127.87	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	51.92	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.898		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
ripol	1530.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1571.00		NIST Webbook
tb	574.26	K	Joback Method
tc	766.81	K	Joback Method
tf	297.75	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.06	J/mol×K	574.26	Joback Method
cpg	576.06	J/mol×K	734.72	Joback Method
cpg	561.18	J/mol×K	702.63	Joback Method
cpg	545.48	J/mol×K	670.54	Joback Method
cpg	528.91	J/mol×K	638.44	Joback Method

cpg	511.45	J/mol×K	606.35	Joback Method
cpg	590.13	J/mol×K	766.81	Joback Method
dvisc	0.0001620	Pa×s	574.26	Joback Method
dvisc	0.0002099	Pa×s	528.17	Joback Method
dvisc	0.0002857	Pa×s	482.09	Joback Method
dvisc	0.0004153	Pa×s	436.00	Joback Method
dvisc	0.0006592	Pa×s	389.92	Joback Method
dvisc	0.0011846	Pa×s	343.83	Joback Method
dvisc	0.0025521	Pa×s	297.75	Joback Method

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=R13777&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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