

Benzene,
1-(1-methylpropyl)-4-(2-methylpropyl)

Inchi:
InChI=1S/C14H22/c1-5-12(4)14-8-6-13(7-9-14)10-11(2)3/h6-9,11-12H,5,10H2,1-4H3

InchiKey:
ABKIAULFUACPBW-UHFFFAOYSA-N

Formula:
C14H22

SMILES:
CCC(C)c1ccc(CC(C)C)cc1

Mol. weight [g/mol]:
190.32

Physical Properties

Property code	Value	Unit	Source
gf	164.90	kJ/mol	Joback Method
hf	-117.79	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	48.92	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.399		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	1306.00		NIST Webbook
ripol	1501.30		NIST Webbook
ripol	1494.00		NIST Webbook
tb	550.50	K	Joback Method
tc	753.79	K	Joback Method
tf	256.48	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.99	J/mol×K	550.50	Joback Method
cpg	461.73	J/mol×K	584.38	Joback Method
cpg	479.47	J/mol×K	618.26	Joback Method
cpg	496.24	J/mol×K	652.14	Joback Method
cpg	512.08	J/mol×K	686.03	Joback Method
cpg	527.03	J/mol×K	719.91	Joback Method
cpg	541.12	J/mol×K	753.79	Joback Method

dvisc	0.0051862	Pa×s	256.48	Joback Method
dvisc	0.0018062	Pa×s	305.48	Joback Method
dvisc	0.0008420	Pa×s	354.49	Joback Method
dvisc	0.0004725	Pa×s	403.49	Joback Method
dvisc	0.0003005	Pa×s	452.49	Joback Method
dvisc	0.0002088	Pa×s	501.50	Joback Method
dvisc	0.0001548	Pa×s	550.50	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=R12501&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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