Benzene, (2-methylpentyl)-

Other names:	(2-Methylpentyl)benzene
	1-Phenyl-2-methylpentane
Inchi:	InChI=1S/C12H18/c1-3-7-11(2)10-12-8-5-4-6-9-12/h4-6,8-9,11H,3,7,10H2,1-2H3
InchiKey:	LFBQYMCKHGBSJY-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCCC(C)Cc1ccccc1
Mol. weight [g/mol]:	162.27
CAS:	39916-61-5

Physical Properties

Property code	Value	Unit	Source
gf	160.13	kJ/mol	Joback Method
hf	-59.76	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.665		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1196.00		NIST Webbook
tb	500.20	K	Joback Method
tc	703.92	K	Joback Method
tf	236.42	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.64	J/mol×K	500.20	Joback Method
cpg	362.97	J/mol×K	534.15	Joback Method
cpg	379.35	J/mol×K	568.11	Joback Method
cpg	394.81	J/mol×K	602.06	Joback Method
cpg	409.40	J/mol×K	636.01	Joback Method
cpg	423.14	J/mol×K	669.96	Joback Method

cpg	436.08	J/mol×K	703.92	Joback Method
dvisc	0.0057131	Pa×s	236.42	Joback Method
dvisc	0.0020964	Pa×s	280.38	Joback Method
dvisc	0.0010095	Pa×s	324.35	Joback Method
dvisc	0.0005788	Pa×s	368.31	Joback Method
dvisc	0.0003736	Pa×s	412.27	Joback Method
dvisc	0.0002624	Pa×s	456.24	Joback Method
dvisc	0.0001961	Pa×s	500.20	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=C39916615&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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