Benzene, (3-methylpentyl)-

Other names: (3-Methylpentyl)benzene
Inchi: InChI=1S/C12H18/c1-3-11(2)9-10-12-7-5-4-6-8-12/h4-8,11H,3,9-10H2,1-2H3
InchiKey: PVXCNEZDIJHZQB-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCC(C)CCc1ccccc1
Mol. weight [g/mol]: 162.27
CAS: 54410-69-4

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	1205.00		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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47631e+01
Coeff. B	-4.20909e+03
Coeff. C	-7.82460e+01
Temperature range (K), min.	369.02
Temperature range (K), max.	523.58

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54410694&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume