Benzene, [2-methyl-1-(1-methylethyl)propyl]-

Other names: Benzene, (1-isopropyl-2-methylpropyl)-
«alpha»,«alpha»-Diisopropyltoluene
(1-Isopropyl-2-methylpropyl)benzene
2,4-Dimethyl-3-phenylpentane
Inchi: InChI=1S/C13H20/c1-10(2)13(11(3)4)12-8-6-5-7-9-12/h5-11,13H,1-4H3
InchiKey: GKGTVJOYFGUPSA-UHFFFAOYSA-N
Formula: C13H20
SMILES: CC(C)C(c1ccccc1)C(C)C
Mol. weight [g/mol]: 176.30
CAS: 21777-84-4

Physical Properties

Property code	Value	Unit	Source
chl	-7364.00	kJ/mol	NIST Webbook
gf	163.67	kJ/mol	Joback Method
hf	-90.96	kJ/mol	Joback Method
hfus	12.90	kJ/mol	Joback Method
hvap	45.64	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	4.082		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1212.00		NIST Webbook
tb	492.16 ± 0.20	K	NIST Webbook
tc	732.01	K	Joback Method
tf	248.70 ± 0.20	K	NIST Webbook
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.47	J/mol×K	522.20	Joback Method
cpg	477.87	J/mol×K	697.04	Joback Method
cpg	462.99	J/mol×K	662.07	Joback Method

cpg	447.16	J/mol×K	627.10	Joback Method
cpg	430.32	J/mol×K	592.14	Joback Method
cpg	412.44	J/mol×K	557.17	Joback Method
cpg	491.84	J/mol×K	732.01	Joback Method
dvisc	0.0001628	Pa×s	522.20	Joback Method
dvisc	0.0002303	Pa×s	471.45	Joback Method
dvisc	0.0003540	Pa×s	420.70	Joback Method
dvisc	0.0006126	Pa×s	369.95	Joback Method
dvisc	0.0012619	Pa×s	319.19	Joback Method
dvisc	0.0034162	Pa×s	268.44	Joback Method
dvisc	0.0147138	Pa×s	217.69	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=C21777844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
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