Benzene, 1-(1-methylethyl)-2-propyl

Inchi: InChI=1S/C12H18/c1-4-7-11-8-5-6-9-12(11)10(2)3/h5-6,8-10H,4,7H2,1-3H3
InchiKey: XNVONTNIANKYKT-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCCc1ccccc1C(C)C
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	150.50	kJ/mol	Joback Method
hf	-71.23	kJ/mol	Joback Method
hfus	16.96	kJ/mol	Joback Method
hvap	44.86	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.763		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
tb	505.18	K	Joback Method
tc	710.08	K	Joback Method
tf	248.94	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.40	J/mol×K	505.18	Joback Method
cpg	363.34	J/mol×K	539.33	Joback Method
cpg	379.40	J/mol×K	573.48	Joback Method
cpg	394.59	J/mol×K	607.63	Joback Method
cpg	408.95	J/mol×K	641.78	Joback Method
cpg	422.51	J/mol×K	675.93	Joback Method
cpg	435.30	J/mol×K	710.08	Joback Method

dvisc	0.0037035	Pa×s	248.94	Joback Method
dvisc	0.0015687	Pa×s	291.65	Joback Method
dvisc	0.0008275	Pa×s	334.35	Joback Method
dvisc	0.0005046	Pa×s	377.06	Joback Method
dvisc	0.0003403	Pa×s	419.77	Joback Method
dvisc	0.0002468	Pa×s	462.47	Joback Method
dvisc	0.0001890	Pa×s	505.18	Joback Method

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=R52868&Units=SI

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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