

(1,4-Dimethylpent-2-enyl)benzene

Inchi:	InChI=1S/C13H18/c1-11(2)9-10-12(3)13-7-5-4-6-8-13/h4-12H,1-3H3/b10-9+
InchiKey:	VKZZGLZQWTWKTP-MDZDMXLPSA-N
Formula:	C13H18
SMILES:	CC(C)C=CC(C)c1ccccc1
Mol. weight [g/mol]:	174.28

Physical Properties

Property code	Value	Unit	Source
gf	246.33	kJ/mol	Joback Method
hf	31.54	kJ/mol	Joback Method
hfus	16.62	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.002		Crippen Method
mvol	165.970	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
tb	526.80	K	Joback Method
tc	741.62	K	Joback Method
tf	227.61	K	Joback Method
vc	0.624	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.58	J/molxK	526.80	Joback Method
cpg	393.73	J/molxK	562.60	Joback Method
cpg	410.74	J/molxK	598.41	Joback Method
cpg	426.69	J/molxK	634.21	Joback Method
cpg	441.61	J/molxK	670.01	Joback Method
cpg	455.59	J/molxK	705.82	Joback Method
cpg	468.67	J/molxK	741.62	Joback Method
dvisc	0.0083154	Paxs	227.61	Joback Method

dvisc	0.0023145	Paxs	277.48	Joback Method
dvisc	0.0009511	Paxs	327.34	Joback Method
dvisc	0.0004945	Paxs	377.20	Joback Method
dvisc	0.0002995	Paxs	427.07	Joback Method
dvisc	0.0002014	Paxs	476.93	Joback Method
dvisc	0.0001461	Paxs	526.80	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=U184979&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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