

Benzene, 1,2,3-trimethyl-4-(2-propenyl)

Inchi:	InChI=1S/C12H16/c1-5-6-12-8-7-9(2)10(3)11(12)4/h5,7-8H,1,6H2,2-4H3
InchiKey:	PVXQYHVKWFSLLL-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	C=CCc1ccc(C)c(C)c1C
Mol. weight [g/mol]:	160.26

Physical Properties

Property code	Value	Unit	Source
gf	221.52	kJ/mol	Joback Method
hf	36.54	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	45.90	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.340		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinsol	1365.00		NIST Webbook
tb	512.26	K	Joback Method
tc	719.31	K	Joback Method
tf	287.22	K	Joback Method
vc	0.581	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.77	J/molxK	512.26	Joback Method
cpg	343.96	J/molxK	546.77	Joback Method
cpg	358.38	J/molxK	581.28	Joback Method
cpg	372.07	J/molxK	615.79	Joback Method
cpg	385.06	J/molxK	650.29	Joback Method
cpg	397.36	J/molxK	684.80	Joback Method
cpg	409.00	J/molxK	719.31	Joback Method
dvisc	0.0012949	Paxs	287.22	Joback Method
dvisc	0.0007818	Paxs	324.73	Joback Method

dvisc	0.0005240	Paxs	362.23	Joback Method
dvisc	0.0003786	Paxs	399.74	Joback Method
dvisc	0.0002892	Paxs	437.25	Joback Method
dvisc	0.0002305	Paxs	474.75	Joback Method
dvisc	0.0001900	Paxs	512.26	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=R59858&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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