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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0005240	Pa×s	362.23	Joback Method
dvisc	0.0003786	Pa×s	399.74	Joback Method
dvisc	0.0002892	Pa×s	437.25	Joback Method
dvisc	0.0002305	Pa×s	474.75	Joback Method
dvisc	0.0001900	Pa×s	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

Latest version available from:
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