Benzene, (1,1,2-trimethylpropyl)-

Other names: 2,3-Dimethyl-2-phenylbutane
(1,1,2-Trimethylpropyl)benzene
Inchi: InChI=1S/C12H18/c1-10(2)12(3,4)11-8-6-5-7-9-11/h5-10H,1-4H3
InchiKey: KOZDEDRKEDUXDC-UHFFFAOYSA-N
Formula: C12H18
SMILES: CC(C)C(C)(C)c1ccccc1
Mol. weight [g/mol]: 162.27
CAS: 26356-11-6

Physical Properties

Property code	Value	Unit	Source
gf	162.97	kJ/mol	Joback Method
hf	-68.51	kJ/mol	Joback Method
hfus	9.94	kJ/mol	Joback Method
hvap	42.90	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.620		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
ripol	1364.00		NIST Webbook
tb	487.15 ± 3.00	K	NIST Webbook
tc	714.13	K	Joback Method
tf	238.84	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.40	J/mol×K	496.97	Joback Method
cpg	367.16	J/mol×K	533.16	Joback Method
cpg	384.69	J/mol×K	569.36	Joback Method
cpg	401.05	J/mol×K	605.55	Joback Method
cpg	416.31	J/mol×K	641.74	Joback Method
cpg	430.53	J/mol×K	677.94	Joback Method

cpg	443.79	J/mol×K	714.13	Joback Method
dvisc	0.0085943	Pa×s	238.84	Joback Method
dvisc	0.0028049	Pa×s	281.86	Joback Method
dvisc	0.0012314	Pa×s	324.88	Joback Method
dvisc	0.0006554	Pa×s	367.90	Joback Method
dvisc	0.0003981	Pa×s	410.93	Joback Method
dvisc	0.0002658	Pa×s	453.95	Joback Method
dvisc	0.0001903	Pa×s	496.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26356116&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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