

Benzene, 2,6-dimethyl-1-(phenylmethyl)-

Inchi:	InChI=1S/C15H16/c1-12-7-6-8-13(2)15(12)11-14-9-4-3-5-10-14/h3-10H,11H2,1-2H3
InchiKey:	OHSBKRHTPKHMQA-UHFFFAOYSA-N
Formula:	C15H16
SMILES:	Cc1cccc(C)c1Cc1ccccc1
Mol. weight [g/mol]:	196.29
CAS:	28122-29-4

Physical Properties

Property code	Value	Unit	Source
gf	280.98	kJ/mol	Joback Method
hf	97.19	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	54.86	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.894		Crippen Method
mcvol	174.690	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	275.40		NIST Webbook
tb	605.92	K	Joback Method
tc	842.62	K	Joback Method
tf	336.69	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.04	J/mol×K	605.92	Joback Method
cpg	438.73	J/mol×K	645.37	Joback Method
cpg	455.19	J/mol×K	684.82	Joback Method
cpg	470.49	J/mol×K	724.27	Joback Method
cpg	484.68	J/mol×K	763.72	Joback Method
cpg	497.83	J/mol×K	803.17	Joback Method
cpg	510.01	J/mol×K	842.62	Joback Method
dvisc	0.0014790	Pa×s	336.69	Joback Method

dvisc	0.0008204	Pa×s	381.56	Joback Method
dvisc	0.0005152	Pa×s	426.43	Joback Method
dvisc	0.0003535	Pa×s	471.31	Joback Method
dvisc	0.0002590	Pa×s	516.18	Joback Method
dvisc	0.0001994	Pa×s	561.05	Joback Method
dvisc	0.0001596	Pa×s	605.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28122294&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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