

Benzene, 2,4-dimethyl-1-(phenylmethyl)-

Inchi:	InChI=1S/C15H16/c1-12-8-9-15(13(2)10-12)11-14-6-4-3-5-7-14/h3-10H,11H2,1-2H3
InchiKey:	CVAMMFFQVDUIEX-UHFFFAOYSA-N
Formula:	C15H16
SMILES:	<chem>Cc1ccc(Cc2ccccc2)c(C)c1</chem>
Mol. weight [g/mol]:	196.29
CAS:	28122-28-3

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	278.50		NIST Webbook
rinpol	278.50		NIST Webbook
tb	569.00 ± 5.00	K	NIST Webbook
tb	569.00 ± 5.00	K	NIST Webbook
tb	556.00 ± 10.00	K	NIST Webbook
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/molxK	605.92	Joback Method
cpg	438.73	J/molxK	645.37	Joback Method
cpg	455.19	J/molxK	684.82	Joback Method
cpg	470.49	J/molxK	724.27	Joback Method
cpg	484.68	J/molxK	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	Paxs	336.69	Joback Method
dvisc	0.0008204	Paxs	381.56	Joback Method
dvisc	0.0005152	Paxs	426.43	Joback Method
dvisc	0.0003535	Paxs	471.31	Joback Method
dvisc	0.0002590	Paxs	516.18	Joback Method
dvisc	0.0001994	Paxs	561.05	Joback Method
dvisc	0.0001596	Paxs	605.92	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=C28122283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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