

Benzene, 1,3-dimethyl-2,4,5-tris-(1-methylethyl)

Inchi:	InChI=1S/C17H28/c1-10(2)15-9-13(7)16(11(3)4)14(8)17(15)12(5)6/h9-12H,1-8H3
InchiKey:	MUYHOROGIUOYPG-UHFFFAOYSA-N
Formula:	C17H28
SMILES:	Cc1cc(C(C)C)c(C(C)C)c(C)c1C(C)C
Mol. weight [g/mol]:	232.40

Physical Properties

Property code	Value	Unit	Source
gf	158.83	kJ/mol	Joback Method
hf	-219.40	kJ/mol	Joback Method
hfus	21.70	kJ/mol	Joback Method
hvap	57.20	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.674		Crippen Method
mcvol	226.630	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
ripol	1819.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1827.00		NIST Webbook
ripol	1819.00		NIST Webbook
tb	633.64	K	Joback Method
tc	835.03	K	Joback Method
tf	312.85	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.85	J/molxK	633.64	Joback Method
cpg	690.17	J/molxK	801.47	Joback Method
cpg	674.20	J/molxK	767.90	Joback Method
cpg	657.30	J/molxK	734.34	Joback Method
cpg	639.47	J/molxK	700.77	Joback Method
cpg	620.66	J/molxK	667.21	Joback Method

cpg	705.26	J/mol×K	835.03	Joback Method
dvisc	0.0001049	Paxs	633.64	Joback Method
dvisc	0.0001374	Paxs	580.17	Joback Method
dvisc	0.0001900	Paxs	526.71	Joback Method
dvisc	0.0002827	Paxs	473.25	Joback Method
dvisc	0.0004656	Paxs	419.78	Joback Method
dvisc	0.0008867	Paxs	366.31	Joback Method
dvisc	0.0021048	Paxs	312.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R555967&Units=SI

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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