

Benzene, 1,4-bis(2,2-dimethylpropyl)-2,3,5,6-tetramethyl-

Other names: Benzene, 1,2,4,5-tetramethyl-3,6-dineopentyl-

Dineopentylidurene

1,2,4,5-Tetramethyl-3,6-di(2,2-dimethylpropyl)benzene

Inchi: InChI=1S/C20H34/c1-13-14(2)18(12-20(8,9)10)16(4)15(3)17(13)11-19(5,6)7/h11-12H2,1

InchiKey: YRQKLQDETHWVBC-UHFFFAOYSA-N

Formula: C20H34

SMILES: Cc1c(C)c(CC(C)(C)C)c(C)c(C)c1CC(C)(C)C

Mol. weight [g/mol]: 274.48

CAS: 33770-83-1

Physical Properties

Property code	Value	Unit	Source
gf	187.46	kJ/mol	Joback Method
hf	-294.45	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	63.11	kJ/mol	Joback Method
ie	7.71	eV	NIST Webbook
log10ws	-7.01		Crippen Method
logp	6.097		Crippen Method
mcvol	268.900	ml/mol	McGowan Method
pc	1236.35	kPa	Joback Method
tb	702.12	K	Joback Method
tc	905.98	K	Joback Method
tf	409.02	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.43	J/molxK	702.12	Joback Method
cpg	865.59	J/molxK	872.00	Joback Method
cpg	849.03	J/molxK	838.03	Joback Method
cpg	831.50	J/molxK	804.05	Joback Method
cpg	812.93	J/molxK	770.07	Joback Method

cpg	793.26	J/molxK	736.10	Joback Method
cpg	881.24	J/molxK	905.98	Joback Method
dvisc	0.0000679	Paxs	702.12	Joback Method
dvisc	0.0000882	Paxs	653.27	Joback Method
dvisc	0.0001195	Paxs	604.42	Joback Method
dvisc	0.0001707	Paxs	555.57	Joback Method
dvisc	0.0002611	Paxs	506.72	Joback Method
dvisc	0.0004376	Paxs	457.87	Joback Method
dvisc	0.0008295	Paxs	409.02	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=C33770831&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
hvac:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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