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

Other names: Benzene, 1,2,3,5-tetramethyl-4,6-dineopentyl-
Dineopentylisodurene
1,2,3,5-Tetramethyl-4,6-di(2,2-dimethylpropyl)benzene

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

InchiKey: NSSMYFQUYITACG-UHFFFAOYSA-N

Formula: C20H34

SMILES: Cc1c(C)c(CC(C)(C)C)c(C)c(CC(C)(C)C)c1C

Mol. weight [g/mol]: 274.48

CAS: 33781-73-6

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	7.72	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/mol×K	702.12	Joback Method
cpg	793.26	J/mol×K	736.10	Joback Method
cpg	812.93	J/mol×K	770.07	Joback Method
cpg	831.50	J/mol×K	804.05	Joback Method
cpg	849.03	J/mol×K	838.03	Joback Method

cpg	865.59	J/mol×K	872.00	Joback Method
cpg	881.24	J/mol×K	905.98	Joback Method
dvisc	0.0008295	Pa×s	409.02	Joback Method
dvisc	0.0004376	Pa×s	457.87	Joback Method
dvisc	0.0002611	Pa×s	506.72	Joback Method
dvisc	0.0001707	Pa×s	555.57	Joback Method
dvisc	0.0001195	Pa×s	604.42	Joback Method
dvisc	0.0000882	Pa×s	653.27	Joback Method
dvisc	0.0000679	Pa×s	702.12	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=C33781736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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