

Benzene, 1-(2,2-dimethyl-1-methylenepropyl)-3,5-dimethyl-

Inchi: InChI=1S/C14H20/c1-10-7-11(2)9-13(8-10)12(3)14(4,5)6/h7-9H,3H2,1-2,4-6H3
InchiKey: CQFFVDLHNWWRNM-UHFFFAOYSA-N
Formula: C14H20
SMILES: C=C(c1cc(C)cc(C)c1)C(C)(C)C
Mol. weight [g/mol]: 188.31
CAS: 146558-41-0

Physical Properties

Property code	Value	Unit	Source
affp	874.30	kJ/mol	NIST Webbook
basg	845.50	kJ/mol	NIST Webbook
gf	242.28	kJ/mol	Joback Method
hf	-11.81	kJ/mol	Joback Method
hfus	15.28	kJ/mol	Joback Method
hvap	48.47	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.363		Crippen Method
mcvol	180.060	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
tb	549.69	K	Joback Method
tc	765.90	K	Joback Method
tf	285.70	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.78	J/molxK	549.69	Joback Method
cpg	444.23	J/molxK	585.72	Joback Method
cpg	461.54	J/molxK	621.76	Joback Method
cpg	477.76	J/molxK	657.79	Joback Method
cpg	492.96	J/molxK	693.83	Joback Method
cpg	507.20	J/molxK	729.86	Joback Method
cpg	520.54	J/molxK	765.90	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=C146558410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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