Benzene, 1-(2,2-dimethyl-1-methylenepropyl)-4-methyl-

Inchi: InChI=1S/C13H18/c1-10-6-8-12(9-7-10)11(2)13(3,4)5/h6-9H,2H2,1,3-5H3
InchiKey: YAHLCBIEBGPTJE-UHFFFAOYSA-N
Formula: C13H18
SMILES: C=C(c1ccc(C)cc1)C(C)(C)C
Mol. weight [g/mol]: 174.28
CAS: 31006-98-1

Physical Properties

Property code	Value	Unit	Source
affp	874.60	kJ/mol	NIST Webbook
basg	845.70	kJ/mol	NIST Webbook
gf	243.49	kJ/mol	Joback Method
hf	20.30	kJ/mol	Joback Method
hfus	13.07	kJ/mol	Joback Method
hvap	45.58	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.054		Crippen Method
mcvol	165.970	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
tb	521.83	K	Joback Method
tc	740.62	K	Joback Method
tf	261.91	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.17	J/mol×K	521.83	Joback Method
cpg	395.40	J/mol×K	558.30	Joback Method
cpg	412.43	J/mol×K	594.76	Joback Method
cpg	428.33	J/mol×K	631.23	Joback Method
cpg	443.16	J/mol×K	667.69	Joback Method
cpg	457.01	J/mol×K	704.16	Joback Method
cpg	469.92	J/mol×K	740.62	Joback Method

Sources

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=C31006981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume