

Benzene, 1-(1,1-dimethylethyl)-4-(1-methylpropyl)

Inchi:	InChI=1S/C14H22/c1-6-11(2)12-7-9-13(10-8-12)14(3,4)5/h7-11H,6H2,1-5H3
InchiKey:	BQOBURPKVKFNKD-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	CCC(C)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	190.32

Physical Properties

Property code	Value	Unit	Source
gf	170.18	kJ/mol	Joback Method
hf	-121.26	kJ/mol	Joback Method
hfus	14.73	kJ/mol	Joback Method
hvap	48.01	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.498		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1499.60		NIST Webbook
ripol	1499.60		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1492.00		NIST Webbook
tb	547.71	K	Joback Method
tc	759.05	K	Joback Method
tf	273.90	K	Joback Method
vc	0.695	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.61	J/molxK	547.71	Joback Method
cpg	465.11	J/molxK	582.93	Joback Method
cpg	483.43	J/molxK	618.16	Joback Method

cpg	500.62	J/molxK	653.38	Joback Method
cpg	516.73	J/molxK	688.60	Joback Method
cpg	531.84	J/molxK	723.83	Joback Method
cpg	546.00	J/molxK	759.05	Joback Method
dvisc	0.0047967	Paxs	273.90	Joback Method
dvisc	0.0017911	Paxs	319.54	Joback Method
dvisc	0.0008556	Paxs	365.17	Joback Method
dvisc	0.0004816	Paxs	410.81	Joback Method
dvisc	0.0003041	Paxs	456.44	Joback Method
dvisc	0.0002087	Paxs	502.08	Joback Method
dvisc	0.0001526	Paxs	547.71	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=R12480&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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