

Benzene, 1,4-dimethyl-2-(1-methylpropyl)

Inchi: InChI=1S/C12H18/c1-5-10(3)12-8-9(2)6-7-11(12)4/h6-8,10H,5H2,1-4H3
InchiKey: YLLKEDBKVUOZDL-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCC(C)c1cc(C)ccc1C
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	140.87	kJ/mol	Joback Method
hf	-82.70	kJ/mol	Joback Method
hfus	16.58	kJ/mol	Joback Method
hvap	45.52	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.817		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
ripol	1191.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1191.00		NIST Webbook
ripol	1191.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1464.00		NIST Webbook
ripol	1452.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1440.00		NIST Webbook
tb	510.16	K	Joback Method
tc	716.23	K	Joback Method
tf	261.46	K	Joback Method
vc	0.594	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.02	J/molxK	510.16	Joback Method
cpg	363.60	J/molxK	544.51	Joback Method
cpg	379.34	J/molxK	578.85	Joback Method
cpg	394.28	J/molxK	613.20	Joback Method
cpg	408.42	J/molxK	647.54	Joback Method
cpg	421.81	J/molxK	681.89	Joback Method
cpg	434.46	J/molxK	716.23	Joback Method
dvisc	0.0025252	Paxs	261.46	Joback Method
dvisc	0.0012079	Paxs	302.91	Joback Method
dvisc	0.0006900	Paxs	344.36	Joback Method
dvisc	0.0004446	Paxs	385.81	Joback Method
dvisc	0.0003119	Paxs	427.26	Joback Method
dvisc	0.0002330	Paxs	468.71	Joback Method
dvisc	0.0001825	Paxs	510.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R52836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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