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

Other names:	1,3-Dimethyl-4-secbutylbenzene
	Benzene, 1,3-dimethyl-4-(1-methylpropyl)
	Benzene, 1,3-dmethyl-4-(1-methylpropyl)
Inchi:	InChI=1S/C12H18/c1-5-10(3)12-7-6-9(2)8-11(12)4/h6-8,10H,5H2,1-4H3
InchiKey:	KAXODKSCABORIG-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCC(C)c1ccc(C)cc1C
Mol. weight [g/mol]:	162.27
CAS:	1483-60-9

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
rinpol	1198.00		NIST Webbook
rinpol	1198.00		NIST Webbook
ripol	1421.40		NIST Webbook
tb	510.16	K	Joback Method
tc	716.23	K	Joback Method
tf	261.46	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.02	J/mol×K	510.16	Joback Method
cpg	421.81	J/mol×K	681.89	Joback Method
cpg	408.42	J/mol×K	647.54	Joback Method

cpg	394.28	J/mol×K	613.20	Joback Method
cpg	379.34	J/mol×K	578.85	Joback Method
cpg	363.60	J/mol×K	544.51	Joback Method
cpg	434.46	J/mol×K	716.23	Joback Method
dvisc	0.0001825	Pa×s	510.16	Joback Method
dvisc	0.0002330	Pa×s	468.71	Joback Method
dvisc	0.0003119	Pa×s	427.26	Joback Method
dvisc	0.0004446	Pa×s	385.81	Joback Method
dvisc	0.0006900	Pa×s	344.36	Joback Method
dvisc	0.0012079	Pa×s	302.91	Joback Method
dvisc	0.0025252	Pa×s	261.46	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1483609&Units=SI

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