Benzene, 1,2-diethyl-3-methyl-

Other names:	Benzene, 2,3-diethyl-1-methyl
	toluene, 2,3-diethyl-
Inchi:	InChI=1S/C11H16/c1-4-10-8-6-7-9(3)11(10)5-2/h6-8H,4-5H2,1-3H3
InchiKey:	LRJOXARIJKBUFE-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCc1cccc(C)c1CC
Mol. weight [g/mol]:	148.24
CAS:	13632-93-4

Physical Properties

Property code	Value	Unit	Source
gf	134.89	kJ/mol	Joback Method
hf	-56.78	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	43.68	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.120		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
ripol	1449.00		NIST Webbook
ripol	1437.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1481.00		NIST Webbook
ripol	1466.00		NIST Webbook
ripol	1451.00		NIST Webbook
tb	487.72	K	Joback Method
tc	692.15	K	Joback Method
tf	265.19	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.47	J/mol×K	487.72	Joback Method
cpg	370.48	J/mol×K	658.08	Joback Method
cpg	358.09	J/mol×K	624.00	Joback Method
cpg	345.01	J/mol×K	589.93	Joback Method
cpg	331.23	J/mol×K	555.86	Joback Method
cpg	316.73	J/mol×K	521.79	Joback Method
cpg	382.22	J/mol×K	692.15	Joback Method
dvisc	0.0002015	Pa×s	487.72	Joback Method
dvisc	0.0002500	Pa×s	450.63	Joback Method
dvisc	0.0003223	Pa×s	413.54	Joback Method
dvisc	0.0004370	Pa×s	376.46	Joback Method
dvisc	0.0006331	Pa×s	339.37	Joback Method
dvisc	0.0010046	Pa×s	302.28	Joback Method
dvisc	0.0018138	Pa×s	265.19	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=C13632934&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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