Benzene, 2,3-diethyl-1-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]: 148.25

Physical Properties

Property code	Value	Unit	Source
af	0.4166		Cheméo Relay (1.0)
gf	134.89	kJ/mol	Joback Method
hf	-44.87	kJ/mol	Cheméo Relay (1.0)
hfus	17.51	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
log10ws	-4.00		Cheméo Relay (1.0)
logp	3.120		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	475.61	K	Cheméo Relay (1.0)
tc	676.36	K	Cheméo Relay (1.0)
tf	240.45	K	Cheméo Relay (1.0)
vc	0.527	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.47	J/mol×K	487.72	Joback Method
cpg	382.22	J/mol×K	692.15	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
dvisc	0.0004370	Pa×s	376.46	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	0.0018138	Pa×s	265.19	Joback Method
dvisc	0.0006331	Pa×s	339.37	Joback Method
dvisc	0.0010046	Pa×s	302.28	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13632934&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
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