

1,3-Diethyl-4-methylbenzene

Other names:	1-Methyl-2,4-di-Ethylbenzene Benzene, 1,3-diethyl-4-methyl Benzene, 2,4-diethyl-1-methyl-
Inchi:	InChI=1S/C11H16/c1-4-10-7-6-9(3)11(5-2)8-10/h6-8H,4-5H2,1-3H3
InchiKey:	PZMJNJDRDKPVLB-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCc1ccc(C)c(CC)c1
Mol. weight [g/mol]:	148.25

Physical Properties

Property code	Value	Unit	Source
af	0.4307		Cheméo Relay (1.0)
gf	134.89	kJ/mol	Joback Method
hf	-44.97	kJ/mol	Cheméo Relay (1.0)
hfus	17.51	kJ/mol	Joback Method
hvap	57.05	kJ/mol	Cheméo Relay (1.0)
ie	8.17	eV	Cheméo Relay (1.0)
log10ws	-4.20		Cheméo Relay (1.0)
logp	3.120		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1149.10		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1148.70		NIST Webbook
rinpol	1149.60		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1154.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1393.00		NIST Webbook
ripol	1393.00		NIST Webbook

ripol	1428.00		NIST Webbook
ripol	1393.10		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1393.10		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1441.00		NIST Webbook
tb	479.11	K	Cheméo Relay (1.0)
tc	675.10	K	Cheméo Relay (1.0)
tf	234.35	K	Cheméo Relay (1.0)
vc	0.538	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	316.73	J/mol×K	521.79	Joback Method
cpg	331.23	J/mol×K	555.86	Joback Method
cpg	345.01	J/mol×K	589.93	Joback Method
cpg	358.09	J/mol×K	624.00	Joback Method
cpg	370.48	J/mol×K	658.08	Joback Method
cpg	382.22	J/mol×K	692.15	Joback Method
dvisc	0.0018138	Pa×s	265.19	Joback Method
dvisc	0.0010046	Pa×s	302.28	Joback Method
dvisc	0.0006331	Pa×s	339.37	Joback Method
dvisc	0.0004370	Pa×s	376.46	Joback Method
dvisc	0.0003223	Pa×s	413.54	Joback Method
dvisc	0.0002500	Pa×s	450.63	Joback Method
dvisc	0.0002015	Pa×s	487.72	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
KDB:	https://www.cheric.org/files/research/kdb/mol/mol693.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1758856&Units=SI

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
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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