

Benzene, 2,4-diethyl-1-methyl-

Other names:	1,3-Diethyl-4-methylbenzene 1-Methyl-2,4-di-Ethylbenzene Benzene, 1,3-diethyl-4-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]:	148.24
CAS:	1758-85-6

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	1148.70		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1149.60		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1149.10		NIST Webbook
ripol	1393.10		NIST Webbook
ripol	1393.00		NIST Webbook
ripol	1393.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1480.00		NIST Webbook

ripol	1468.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1393.10		NIST Webbook
tb	487.72	K	Joback Method
tc	692.15	K	Joback Method
tf	265.19	K	Joback Method
vc	0.543	m ³ /kmol	Joback Method

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	Paxs	265.19	Joback Method
dvisc	0.0010046	Paxs	302.28	Joback Method
dvisc	0.0006331	Paxs	339.37	Joback Method
dvisc	0.0004370	Paxs	376.46	Joback Method
dvisc	0.0003223	Paxs	413.54	Joback Method
dvisc	0.0002500	Paxs	450.63	Joback Method
dvisc	0.0002015	Paxs	487.72	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1758856&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Joback Method:

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

KDB:

<https://www.cheric.org/files/research/kdb/mol/mol693.mol>

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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