

BENZENE, 1-METHYL-4-(1-METHYLPROPYL)-

Other names:	1-Methyl-4-(1-methylpropyl)-benzene 1-Methyl-4-sec-butylbenzene
Inchi:	InChI=1S/C11H16/c1-4-10(3)11-7-5-9(2)6-8-11/h5-8,10H,4H2,1-3H3
InchiKey:	LWCFXYMSEGQWNB-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCC(C)c1ccc(C)cc1
Mol. weight [g/mol]:	148.25
CAS:	1595-16-0

Physical Properties

Property code	Value	Unit	Source
af	0.3793		Cheméo Relay (1.0)
gf	142.08	kJ/mol	Joback Method
hf	-59.89	kJ/mol	Cheméo Relay (1.0)
hfus	14.37	kJ/mol	Joback Method
hvap	51.85	kJ/mol	Cheméo Relay (1.0)
ie	8.27	eV	Cheméo Relay (1.0)
log10ws	-4.17		Cheméo Relay (1.0)
logp	3.509		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1088.70		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1088.70		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
ripol	1315.40		NIST Webbook
ripol	1315.40		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1315.00		NIST Webbook
tb	470.00 ± 5.00	K	NIST Webbook
tb	476.00 ± 5.00	K	NIST Webbook
tb	469.00 ± 5.00	K	NIST Webbook
tb	475.00 ± 4.00	K	NIST Webbook

tb	467.00 ± 5.00	K	NIST Webbook
tc	670.76	K	Cheméo Relay (1.0)
tf	232.00	K	Cheméo Relay (1.0)
vc	0.519	m ³ /kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.93	J/mol×K	482.30	Joback Method
cpg	317.03	J/mol×K	516.94	Joback Method
cpg	332.27	J/mol×K	551.59	Joback Method
cpg	346.68	J/mol×K	586.23	Joback Method
cpg	360.30	J/mol×K	620.88	Joback Method
cpg	373.16	J/mol×K	655.52	Joback Method
cpg	385.28	J/mol×K	690.17	Joback Method
dvisc	0.0036688	Pa×s	237.67	Joback Method
dvisc	0.0015812	Pa×s	278.44	Joback Method
dvisc	0.0008449	Pa×s	319.21	Joback Method
dvisc	0.0005204	Pa×s	359.99	Joback Method
dvisc	0.0003537	Pa×s	400.76	Joback Method
dvisc	0.0002582	Pa×s	441.53	Joback Method
dvisc	0.0001987	Pa×s	482.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42798e+01
Coeff. B	-3.85077e+03
Coeff. C	-7.15800e+01
Temperature range (K), min.	346.79
Temperature range (K), max.	500.95

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1595160&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
pvap:	Vapor 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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