

Benzene, (2-methylbutyl)-

Other names:	(2-Methylbutyl)benzene 1-Phenyl-2-methylbutane 2-Methyl-1-phenylbutane Butane, 2-methyl-1-phenyl-
Inchi:	InChI=1S/C11H16/c1-3-10(2)9-11-7-5-4-6-8-11/h4-8,10H,3,9H2,1-2H3
InchiKey:	IFDLFCDWOFLKEB-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCC(C)Cc1ccccc1
Mol. weight [g/mol]:	148.24
CAS:	3968-85-2

Physical Properties

Property code	Value	Unit	Source
gf	151.71	kJ/mol	Joback Method
hf	-39.12	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	41.97	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.275		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1105.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1100.70		NIST Webbook
rinpol	1102.10		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1102.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1309.30		NIST Webbook

ripol	1309.30		NIST Webbook
tb	469.15 ± 2.00	K	NIST Webbook
tb	462.65 ± 2.00	K	NIST Webbook
tb	469.25 ± 0.40	K	NIST Webbook
tb	468.00 ± 6.00	K	NIST Webbook
tb	467.00 ± 6.00	K	NIST Webbook
tc	683.92	K	Joback Method
tf	225.15	K	Joback Method
vc	0.537	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.07	J/mol×K	477.32	Joback Method
cpg	316.59	J/mol×K	511.75	Joback Method
cpg	332.19	J/mol×K	546.19	Joback Method
cpg	346.91	J/mol×K	580.62	Joback Method
cpg	360.78	J/mol×K	615.05	Joback Method
cpg	373.84	J/mol×K	649.49	Joback Method
cpg	386.13	J/mol×K	683.92	Joback Method
dvisc	0.0057730	Paxs	225.15	Joback Method
dvisc	0.0021444	Paxs	267.18	Joback Method
dvisc	0.0010427	Paxs	309.21	Joback Method
dvisc	0.0006024	Paxs	351.24	Joback Method
dvisc	0.0003914	Paxs	393.26	Joback Method
dvisc	0.0002764	Paxs	435.29	Joback Method
dvisc	0.0002075	Paxs	477.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42983e+01
Coeff. B	-3.85816e+03
Coeff. C	-7.15800e+01
Temperature range (K), min.	346.95
Temperature range (K), max.	500.89

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=C3968852&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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