

Benzene, 1-bromo-3-methoxy-

Other names:	Anisole, m-bromo- m-Anisyl bromide m-Bromoanisole 3-Bromoanisole m-Bromomethoxybenzene m-Bromophenyl methyl ether m-Methoxybromobenzene 3-Methoxybromobenzene 3-Methoxy-1-bromobenzene m-Methoxyphenyl bromide 3-Methoxyphenyl bromide 3-Bromoanisol 1-Bromo-3-methoxybenzene NSC 82293
Inchi:	InChI=1S/C7H7BrO/c1-9-7-4-2-3-6(8)5-7/h2-5H,1H3
InchiKey:	PLDWAJLZAAHOGG-UHFFFAOYSA-N
Formula:	C7H7BrO
SMILES:	COc1cccc(Br)c1
Mol. weight [g/mol]:	187.03
CAS:	2398-37-0

Physical Properties

Property code	Value	Unit	Source
gf	20.16	kJ/mol	Joback Method
hf	-68.64	kJ/mol	Joback Method
hfus	14.01	kJ/mol	Joback Method
hvac	58.00 ± 1.20	kJ/mol	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-2.75		Crippen Method
logp	2.458		Crippen Method
mccvol	109.100	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1149.00		NIST Webbook
tb	483.70	K	NIST Webbook

tb	483.50 ± 0.50	K	NIST Webbook
tc	711.08	K	Joback Method
tf	289.62	K	Joback Method
vc	0.400	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.04	J/mol×K	479.80	Joback Method
cpg	204.18	J/mol×K	518.35	Joback Method
cpg	213.74	J/mol×K	556.89	Joback Method
cpg	222.71	J/mol×K	595.44	Joback Method
cpg	231.12	J/mol×K	633.98	Joback Method
cpg	238.99	J/mol×K	672.53	Joback Method
cpg	246.33	J/mol×K	711.08	Joback Method
dvisc	0.0016504	Paxs	289.62	Joback Method
dvisc	0.0010390	Paxs	321.32	Joback Method
dvisc	0.0007108	Paxs	353.01	Joback Method
dvisc	0.0005176	Paxs	384.71	Joback Method
dvisc	0.0003956	Paxs	416.41	Joback Method
dvisc	0.0003141	Paxs	448.10	Joback Method
dvisc	0.0002571	Paxs	479.80	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2398370&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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