3-BROMO-ORTHO-XYLENE

Other names: 1-Bromo-2,3-dimethylbenzene
3-Bromo-1,2-dimethylbenzene
3-Bromo-o-xylene
Inchi: InChI=1S/C8H9Br/c1-6-4-3-5-8(9)7(6)2/h3-5H,1-2H3
InchiKey: WLPXNBYWDDYJTN-UHFFFAOYSA-N
Formula: C8H9Br
SMILES: Cc1cccc(Br)c1C
Mol. weight [g/mol]: 185.06
CAS: 576-23-8

Physical Properties

Property code	Value	Unit	Source
af	0.3415		Cheméo Relay (1.0)
gf	123.95	kJ/mol	Joback Method
hf	48.14	kJ/mol	Cheméo Relay (1.0)
hfus	15.02	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-3.88		Cheméo Relay (1.0)
logp	3.066		Crippen Method
mcvol	117.320	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	487.00	K	NIST Webbook
tb	484.50 ± 1.50	K	NIST Webbook
tb	487.20	K	NIST Webbook
tc	706.86	K	Cheméo Relay (1.0)
tf	303.16	K	Cheméo Relay (1.0)
vc	0.420	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.91	J/mol×K	485.24	Joback Method
cpg	224.18	J/mol×K	523.77	Joback Method

cpg	234.76	J/mol×K	562.30	Joback Method
cpg	244.68	J/mol×K	600.83	Joback Method
cpg	253.98	J/mol×K	639.37	Joback Method
cpg	262.68	J/mol×K	677.90	Joback Method
cpg	270.81	J/mol×K	716.43	Joback Method
dvisc	0.0016069	Pa×s	291.18	Joback Method
dvisc	0.0010357	Pa×s	323.52	Joback Method
dvisc	0.0007230	Pa×s	355.87	Joback Method
dvisc	0.0005358	Pa×s	388.21	Joback Method
dvisc	0.0004159	Pa×s	420.55	Joback Method
dvisc	0.0003347	Pa×s	452.90	Joback Method
dvisc	0.0002772	Pa×s	485.24	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41286e+01
Coeff. B	-3.90514e+03
Coeff. C	-7.65780e+01
Temperature range (K), min.	358.72
Temperature range (K), max.	519.48

Sources

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=C576238&Units=SI

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

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