2-Bromo-p-cymene

Other names: Benzene, 2-bromo-1-methyl-4-(1-methylethyl)-
Inchi: InChI=1S/C10H13Br/c1-7(2)9-5-4-8(3)10(11)6-9/h4-7H,1-3H3
InchiKey: SPQXEZCUUYJJQL-UHFFFAOYSA-N
Formula: C10H13Br
SMILES: Cc1ccc(C(C)C)cc1Br
Mol. weight [g/mol]: 213.11
CAS: 2437-76-5

Physical Properties

Property code	Value	Unit	Source
gf	138.35	kJ/mol	Joback Method
hf	-15.09	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	47.50	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.881		Crippen Method
mcvol	145.500	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	507.45 ± 0.50	K	NIST Webbook
tb	507.50	K	NIST Webbook
tc	758.86	K	Joback Method
tf	298.72	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.50	J/mol×K	530.56	Joback Method
cpg	312.40	J/mol×K	568.61	Joback Method
cpg	325.46	J/mol×K	606.66	Joback Method
cpg	337.72	J/mol×K	644.71	Joback Method
cpg	349.20	J/mol×K	682.76	Joback Method
cpg	359.96	J/mol×K	720.81	Joback Method
cpg	370.02	J/mol×K	758.86	Joback Method

dvisc	0.0020742	Pa×s	298.72	Joback Method
dvisc	0.0011645	Pa×s	337.36	Joback Method
dvisc	0.0007362	Pa×s	376.00	Joback Method
dvisc	0.0005069	Pa×s	414.64	Joback Method
dvisc	0.0003720	Pa×s	453.28	Joback Method
dvisc	0.0002865	Pa×s	491.92	Joback Method
dvisc	0.0002293	Pa×s	530.56	Joback Method
hvapt	50.20	kJ/mol	455.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.20	K	1.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2437765&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure

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