METHYL P-BROMOBENZOATE

Other names:	4-Bromobenzoic acid, methyl ester
	Benzoic acid, p-bromo-, methyl ester
	methyl 4-bromobenzoate
	p-Bromobenzoic acid, methyl ester
Inchi:	InChI=1S/C8H7BrO2/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5H,1H3
InchiKey:	CZNGTXVOZOWWKM-UHFFFAOYSA-N
Formula:	C8H7BrO2
SMILES:	COC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]:	215.05

Physical Properties

Property code	Value	Unit	Source
af	0.4810		Cheméo Relay (1.0)
hf	-257.50	kJ/mol	Cheméo Relay (1.0)
hfus	18.20	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Cheméo Relay (1.0)
ie	9.47	eV	NIST Webbook
log10ws	-3.34		Cheméo Relay (1.0)
logp	2.236		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	1336.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1336.00		NIST Webbook
tb	524.05	K	Cheméo Relay (1.0)
tc	734.12	K	Cheméo Relay (1.0)
tf	351.22	K	The influence of the halogen size in the volatility and melting of methyl p-halobenzoic esters and of their parent acids
vc	0.439	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.83	J/mol×K	556.55	Joback Method
cpg	257.12	J/mol×K	595.93	Joback Method
cpg	266.74	J/mol×K	635.32	Joback Method
cpg	275.70	J/mol×K	674.70	Joback Method
cpg	284.02	J/mol×K	714.09	Joback Method
cpg	291.72	J/mol×K	753.47	Joback Method
cpg	298.81	J/mol×K	792.86	Joback Method
dvisc	0.0015564	Pa×s	350.82	Joback Method
dvisc	0.0010113	Pa×s	385.11	Joback Method
dvisc	0.0007051	Pa×s	419.40	Joback Method
dvisc	0.0005191	Pa×s	453.69	Joback Method
dvisc	0.0003990	Pa×s	487.97	Joback Method
dvisc	0.0003175	Pa×s	522.26	Joback Method
dvisc	0.0002598	Pa×s	556.55	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The influence of the halogen size in the volatility and melting of methyl p-halobenzoic esters and of their parent acids: https://www.doi.org/10.1016/j.jct.2012.07.027

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C619421&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
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