2-Bromo-5-methylbenzoic acid

Inchi: InChI=1S/C8H7BrO2/c1-5-2-3-7(9)6(4-5)8(10)11/h2-4H,1H3,(H,10,11)
InchiKey: ZXMISUUIYPFORW-UHFFFAOYSA-N
Formula: C8H7BrO2
SMILES: Cc1ccc(Br)c(C(=O)O)c1
Mol. weight [g/mol]: 215.04
CAS: 6967-82-4

Physical Properties

Property code	Value	Unit	Source
gf	-141.79	kJ/mol	Joback Method
hf	-233.34	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	66.86	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.456		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	631.29	K	Joback Method
tc	852.05	K	Joback Method
tf	401.93	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.03	J/mol×K	631.29	Joback Method
cpg	272.16	J/mol×K	668.08	Joback Method
cpg	279.75	J/mol×K	704.88	Joback Method
cpg	286.82	J/mol×K	741.67	Joback Method
cpg	293.39	J/mol×K	778.46	Joback Method
cpg	299.50	J/mol×K	815.26	Joback Method
cpg	305.18	J/mol×K	852.05	Joback Method
dvisc	0.0018526	Pa×s	401.93	Joback Method
dvisc	0.0009189	Pa×s	440.16	Joback Method

dvisc	0.0005098	Pa×s	478.38	Joback Method
dvisc	0.0003086	Pa×s	516.61	Joback Method
dvisc	0.0002002	Pa×s	554.84	Joback Method
dvisc	0.0001373	Pa×s	593.06	Joback Method
dvisc	0.0000986	Pa×s	631.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6967824&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume