(E)-3-(2-Bromophenyl)propenoic acid

Other names:	2-Bromocinnamic acid
	o-Bromocinnamic acid
	2-Propenoic acid, 3-(2-bromophenyl)-
	Cinnamic acid, o-bromo-
Inchi:	InChI=1S/C9H7BrO2/c10-8-4-2-1-3-7(8)5-6-9(11)12/h1-6H,(H,11,12)/b6-5+
InchiKey:	OMHDOOAFLCMRFX-AATRIKPKSA-N
Formula:	C9H7BrO2
SMILES:	O=C(O)C=Cc1ccccc1Br
Mol. weight [g/mol]:	227.06
CAS:	7499-56-1

Physical Properties

Property code	Value	Unit	Source
chs	-4130.00	kJ/mol	NIST Webbook
gf	-43.52	kJ/mol	Joback Method
hf	-125.29	kJ/mol	Joback Method
hfs	-305.20	kJ/mol	NIST Webbook
hfus	23.89	kJ/mol	Joback Method
hvap	68.38	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
log10ws	-2.98		Crippen Method
logp	2.547		Crippen Method
mcvol	134.550	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	653.35	K	Joback Method
tc	878.21	K	Joback Method
tf	395.60	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.45	J/mol×K	653.35	Joback Method
cpg	297.87	J/mol×K	690.83	Joback Method

cpg	305.65	J/mol×K	728.30	Joback Method
cpg	312.86	J/mol×K	765.78	Joback Method
cpg	319.54	J/mol×K	803.25	Joback Method
cpg	325.75	J/mol×K	840.73	Joback Method
cpg	331.55	J/mol×K	878.21	Joback Method
dvisc	0.0020723	Pa×s	395.60	Joback Method
dvisc	0.0009003	Pa×s	438.56	Joback Method
dvisc	0.0004539	Pa×s	481.52	Joback Method
dvisc	0.0002560	Pa×s	524.48	Joback Method
dvisc	0.0001575	Pa×s	567.43	Joback Method
dvisc	0.0001037	Pa×s	610.39	Joback Method
dvisc	0.0000722	Pa×s	653.35	Joback Method

Sources

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=C7499561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume