

3-Bromocinnamic acid

Other names:	m-Bromocinnamic acid trans-3-Bromocinnamic acid 2-Propenoic acid, 3-(3-bromophenyl)- BW A800U Cinnamic acid, m-bromo-
Inchi:	InChI=1S/C9H7BrO2/c10-8-3-1-2-7(6-8)4-5-9(11)12/h1-6H,(H,11,12)/b5-4+
InchiKey:	YEMUSDCFQUBPAL-SNAWJCMRSA-N
Formula:	C9H7BrO2
SMILES:	O=C(O)C=Cc1cccc(Br)c1
Mol. weight [g/mol]:	227.06
CAS:	32862-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-43.52	kJ/mol	Joback Method
hf	-125.29	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	68.38	kJ/mol	Joback Method
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/molxK	653.35	Joback Method
cpg	297.87	J/molxK	690.83	Joback Method
cpg	305.65	J/molxK	728.30	Joback Method
cpg	312.86	J/molxK	765.78	Joback Method

cpg	319.54	J/molxK	803.25	Joback Method
cpg	325.75	J/molxK	840.73	Joback Method
cpg	331.55	J/molxK	878.21	Joback Method
dvisc	0.0020723	Paxs	395.60	Joback Method
dvisc	0.0009003	Paxs	438.56	Joback Method
dvisc	0.0004539	Paxs	481.52	Joback Method
dvisc	0.0002560	Paxs	524.48	Joback Method
dvisc	0.0001575	Paxs	567.43	Joback Method
dvisc	0.0001037	Paxs	610.39	Joback Method
dvisc	0.0000722	Paxs	653.35	Joback Method

Sources

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=C32862978&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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