2-Propenal, 2-bromo-3-phenyl-

Other names:	Alphabrocine
	B 37
	«alpha»-Bromocinnamaldehyde
	«alpha»-Bromocinnamic Aldehyde
	Cinnamaldehyde, «alpha»-bromo-
	2-bromocinnamaldehyde
Inchi:	InChI=1S/C9H7BrO/c10-9(7-11)6-8-4-2-1-3-5-8/h1-7H/b9-6-
InchiKey:	WQRWNOKNRHCLHV-TWGQIWQCSA-N
Formula:	C9H7BrO
SMILES:	O=CC(Br)=Cc1ccccc1
Mol. weight [g/mol]:	211.06
CAS:	5443-49-2

Physical Properties

Property code	Value	Unit	Source
gf	123.78	kJ/mol	Joback Method
hf	55.62	kJ/mol	Joback Method
hfus	19.57	kJ/mol	Joback Method
hvap	51.10	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.621		Crippen Method
mcvol	128.680	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
tb	550.86	K	Joback Method
tc	794.52	K	Joback Method
tf	300.37	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.48	J/mol×K	550.86	Joback Method
cpg	262.49	J/mol×K	591.47	Joback Method
cpg	272.56	J/mol×K	632.08	Joback Method

cpg	281.75	J/mol×K	672.69	Joback Method
cpg	290.16	J/mol×K	713.30	Joback Method
cpg	297.86	J/mol×K	753.91	Joback Method
cpg	304.94	J/mol×K	794.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5443492&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

Legend

cpg:	Ideal gas heat capacity
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