«alpha»,«beta»-Dibromohydrocinnamic acid

Other names:	2,3-Dibromo-3-phenylpropionic acid
	2,3-Dibromohydrocinnamic acid
	Benzenepropanoic acid, «alpha»,«beta»-dibromo-
	Hydrocinnamic acid, «alpha»,«beta»-dibromo-
	2,3-Dibromo-3-phenylpropanoic acid
	Propionic acid, 2,3-dibromo-3-phenyl-
	alpha,beta-Dibromohydrocinnamic acid
Inchi:	InChI=1S/C9H8Br2O2/c10-7(8(11)9(12)13)6-4-2-1-3-5-6/h1-5,7-8H,(H,12,13)
InchiKey:	FXJWTHBNVZNQQP-UHFFFAOYSA-N
Formula:	C9H8Br2O2
SMILES:	O=C(O)C(Br)C(Br)c1ccccc1
Mol. weight [g/mol]:	307.97
CAS:	6286-30-2

Physical Properties

Property code	Value	Unit	Source
gf	-104.67	kJ/mol	Joback Method
hf	-215.27	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	73.42	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.971		Crippen Method
mcvol	156.350	ml/mol	McGowan Method
pc	4809.16	kPa	Joback Method
tb	709.49	K	Joback Method
tc	944.19	K	Joback Method
tf	417.96	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.09	J/mol×K	709.49	Joback Method
cpg	379.06	J/mol×K	905.08	Joback Method

cpg	373.02	J/mol×K	865.96	Joback Method
cpg	366.47	J/mol×K	826.84	Joback Method
cpg	359.34	J/mol×K	787.72	Joback Method
cpg	351.57	J/mol×K	748.61	Joback Method
cpg	384.66	J/mol×K	944.19	Joback Method
dvisc	0.0000544	Pa×s	709.49	Joback Method
dvisc	0.0000806	Pa×s	660.90	Joback Method
dvisc	0.0001273	Pa×s	612.31	Joback Method
dvisc	0.0002173	Pa×s	563.73	Joback Method
dvisc	0.0004106	Pa×s	515.14	Joback Method
dvisc	0.0008856	Pa×s	466.55	Joback Method
dvisc	0.0022841	Pa×s	417.96	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=C6286302&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