Ethanone, 2-bromo-1-(3-bromophenyl)-

Other names: 3-Bromophenacyl bromide
Inchi: InChI=1S/C8H6Br2O/c9-5-8(11)6-2-1-3-7(10)4-6/h1-4H,5H2
InchiKey: MZBXSQBQPJWECM-UHFFFAOYSA-N
Formula: C8H6Br2O
SMILES: O=C(CBr)c1cccc(Br)c1
Mol. weight [g/mol]: 277.94
CAS: 18523-22-3

Physical Properties

Property code	Value	Unit	Source
gf	18.98	kJ/mol	Joback Method
hf	-43.31	kJ/mol	Joback Method
hfus	22.30	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.027		Crippen Method
mcvol	136.390	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
tb	600.29	K	Joback Method
tc	854.10	K	Joback Method
tf	388.39	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.27	J/mol×K	600.29	Joback Method
cpg	264.55	J/mol×K	642.59	Joback Method
cpg	273.04	J/mol×K	684.89	Joback Method
cpg	280.79	J/mol×K	727.20	Joback Method
cpg	287.88	J/mol×K	769.50	Joback Method
cpg	294.37	J/mol×K	811.80	Joback Method
cpg	300.32	J/mol×K	854.10	Joback Method
dvisc	0.0016776	Pa×s	388.39	Joback Method

dvisc	0.0011251	Pa×s	423.71	Joback Method
dvisc	0.0008024	Pa×s	459.02	Joback Method
dvisc	0.0006005	Pa×s	494.34	Joback Method
dvisc	0.0004672	Pa×s	529.66	Joback Method
dvisc	0.0003750	Pa×s	564.97	Joback Method
dvisc	0.0003089	Pa×s	600.29	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=C18523223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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