4-Bromobenzoic acid, phenyl ester

Inchi: InChI=1S/C13H9BrO2/c14-11-8-6-10(7-9-11)13(15)16-12-4-2-1-3-5-12/h1-9H
InchiKey: GKOPHSXEQSIHQE-UHFFFAOYSA-N
Formula: C13H9BrO2
SMILES: O=C(Oc1ccccc1)c1ccc(Br)cc1
Mol. weight [g/mol]: 277.11

Physical Properties

Property code	Value	Unit	Source
gf	54.17	kJ/mol	Joback Method
hf	-68.53	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	65.34	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.668		Crippen Method
mcvol	171.450	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	1901.00		NIST Webbook
tb	697.63	K	Joback Method
tc	958.04	K	Joback Method
tf	433.59	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.78	J/mol×K	697.63	Joback Method
cpg	412.50	J/mol×K	741.03	Joback Method
cpg	424.05	J/mol×K	784.43	Joback Method
cpg	434.51	J/mol×K	827.84	Joback Method
cpg	443.93	J/mol×K	871.24	Joback Method
cpg	452.40	J/mol×K	914.64	Joback Method
cpg	459.97	J/mol×K	958.04	Joback Method
dvisc	0.0010570	Pa×s	433.59	Joback Method
dvisc	0.0006618	Pa×s	477.60	Joback Method

dvisc	0.0004484	Pa×s	521.60	Joback Method
dvisc	0.0003228	Pa×s	565.61	Joback Method
dvisc	0.0002437	Pa×s	609.62	Joback Method
dvisc	0.0001911	Pa×s	653.62	Joback Method
dvisc	0.0001545	Pa×s	697.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299026&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume