

3-Bromobenzoic acid, phenyl ester

Inchi:	InChI=1S/C13H9BrO2/c14-11-6-4-5-10(9-11)13(15)16-12-7-2-1-3-8-12/h1-9H
InchiKey:	DPXSFDIOGXVWPF-UHFFFAOYSA-N
Formula:	C13H9BrO2
SMILES:	O=C(Oc1ccccc1)c1cccc(Br)c1
Mol. weight [g/mol]:	277.11
CAS:	82723-17-9

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	1959.00		NIST Webbook
rinpol	1959.00		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/molxK	697.63	Joback Method
cpg	452.40	J/molxK	914.64	Joback Method
cpg	443.93	J/molxK	871.24	Joback Method
cpg	434.51	J/molxK	827.84	Joback Method
cpg	424.05	J/molxK	784.43	Joback Method
cpg	412.50	J/molxK	741.03	Joback Method
cpg	459.97	J/molxK	958.04	Joback Method

dvisc	0.0001545	Paxs	697.63	Joback Method
dvisc	0.0001911	Paxs	653.62	Joback Method
dvisc	0.0002437	Paxs	609.62	Joback Method
dvisc	0.0003228	Paxs	565.61	Joback Method
dvisc	0.0004484	Paxs	521.60	Joback Method
dvisc	0.0006618	Paxs	477.60	Joback Method
dvisc	0.0010570	Paxs	433.59	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=C82723179&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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