Benzoic acid, (3-bromophenyl)methyl ester

Inchi: InChI=1S/C14H11BrO2/c15-13-8-4-5-11(9-13)10-17-14(16)12-6-2-1-3-7-12/h1-9H,10H2
InchiKey: WXYMOFXETVOVOQ-UHFFFAOYSA-N
Formula: C14H11BrO2
SMILES: O=C(OCc1cccc(Br)c1)c1ccccc1
Mol. weight [g/mol]: 291.14

Physical Properties

Property code	Value	Unit	Source
gf	62.59	kJ/mol	Joback Method
hf	-89.17	kJ/mol	Joback Method
hfus	27.78	kJ/mol	Joback Method
hvap	67.56	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.806		Crippen Method
mcvol	185.540	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	2124.00		NIST Webbook
tb	720.51	K	Joback Method
tc	974.88	K	Joback Method
tf	444.86	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.38	J/mol×K	720.51	Joback Method
cpg	463.65	J/mol×K	762.90	Joback Method
cpg	475.74	J/mol×K	805.30	Joback Method
cpg	486.72	J/mol×K	847.69	Joback Method
cpg	496.67	J/mol×K	890.09	Joback Method
cpg	505.64	J/mol×K	932.48	Joback Method
cpg	513.71	J/mol×K	974.88	Joback Method
dvisc	0.0009888	Pa×s	444.86	Joback Method
dvisc	0.0006098	Pa×s	490.80	Joback Method

dvisc	0.0004085	Pa×s	536.74	Joback Method
dvisc	0.0002915	Pa×s	582.68	Joback Method
dvisc	0.0002185	Pa×s	628.63	Joback Method
dvisc	0.0001704	Pa×s	674.57	Joback Method
dvisc	0.0001371	Pa×s	720.51	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=U368727&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume