3-Bromobenzoic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C12H15BrO2/c1-8(2)9(3)15-12(14)10-5-4-6-11(13)7-10/h4-9H,1-3H3
InchiKey: ZFQKOCHXRZEJJJ-UHFFFAOYSA-N
Formula: C12H15BrO2
SMILES: CC(C)C(C)OC(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 271.15

Physical Properties

Property code	Value	Unit	Source
gf	-71.54	kJ/mol	Joback Method
hf	-294.98	kJ/mol	Joback Method
hfus	21.51	kJ/mol	Joback Method
hvap	60.06	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.650		Crippen Method
mcvol	181.120	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	1682.00		NIST Webbook
tb	647.19	K	Joback Method
tc	875.08	K	Joback Method
tf	365.90	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.91	J/mol×K	647.19	Joback Method
cpg	449.28	J/mol×K	685.17	Joback Method
cpg	462.69	J/mol×K	723.15	Joback Method
cpg	475.16	J/mol×K	761.14	Joback Method
cpg	486.75	J/mol×K	799.12	Joback Method
cpg	497.48	J/mol×K	837.10	Joback Method
cpg	507.38	J/mol×K	875.08	Joback Method
dvisc	0.0019092	Pa×s	365.90	Joback Method
dvisc	0.0009792	Pa×s	412.78	Joback Method

dvisc	0.0005755	Pa×s	459.66	Joback Method
dvisc	0.0003732	Pa×s	506.55	Joback Method
dvisc	0.0002604	Pa×s	553.43	Joback Method
dvisc	0.0001922	Pa×s	600.31	Joback Method
dvisc	0.0001483	Pa×s	647.19	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=U355180&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