

3-Bromobenzoic acid, 3-methylbutyl ester

Inchi:	InChI=1S/C12H15BrO2/c1-9(2)6-7-15-12(14)10-4-3-5-11(13)8-10/h3-5,8-9H,6-7H2,1-2H1
InchiKey:	BULPKMWHBGPVIB-UHFFFAOYSA-N
Formula:	C12H15BrO2
SMILES:	CC(C)CCOC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	271.15

Physical Properties

Property code	Value	Unit	Source
gf	-69.10	kJ/mol	Joback Method
hf	-289.70	kJ/mol	Joback Method
hfus	25.04	kJ/mol	Joback Method
hvap	60.45	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.652		Crippen Method
mcvol	181.120	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpola	1755.00		NIST Webbook
tb	647.63	K	Joback Method
tc	870.96	K	Joback Method
tf	380.90	K	Joback Method
vc	0.679	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.41	J/molxK	647.63	Joback Method
cpg	448.45	J/molxK	684.85	Joback Method
cpg	461.58	J/molxK	722.07	Joback Method
cpg	473.83	J/molxK	759.29	Joback Method
cpg	485.23	J/molxK	796.52	Joback Method
cpg	495.82	J/molxK	833.74	Joback Method
cpg	505.62	J/molxK	870.96	Joback Method
dvisc	0.0015681	Paxs	380.90	Joback Method
dvisc	0.0008781	Paxs	425.36	Joback Method

dvisc	0.0005487	Paxs	469.81	Joback Method
dvisc	0.0003719	Paxs	514.26	Joback Method
dvisc	0.0002682	Paxs	558.72	Joback Method
dvisc	0.0002030	Paxs	603.17	Joback Method
dvisc	0.0001596	Paxs	647.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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