

Methyl 3-bromomethylbenzoate

Other names:	m-Carbomethoxybenzyl bromide
Inchi:	InChI=1S/C9H9BrO2/c1-12-9(11)8-4-2-3-7(5-8)6-10/h2-5H,6H2,1H3
InchiKey:	YUHSMQQNPRLEEJ-UHFFFAOYSA-N
Formula:	C9H9BrO2
SMILES:	<chem>COC(=O)c1cccc(CBr)c1</chem>
Mol. weight [g/mol]:	229.07
CAS:	1129-28-8

Physical Properties

Property code	Value	Unit	Source
gf	-91.92	kJ/mol	Joback Method
hf	-222.50	kJ/mol	Joback Method
hfus	20.79	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.368		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	579.43	K	Joback Method
tc	811.07	K	Joback Method
tf	362.09	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.08	J/molxK	579.43	Joback Method
cpg	340.71	J/molxK	772.46	Joback Method
cpg	332.17	J/molxK	733.85	Joback Method
cpg	322.96	J/molxK	695.25	Joback Method
cpg	313.06	J/molxK	656.64	Joback Method
cpg	302.44	J/molxK	618.04	Joback Method
cpg	348.60	J/molxK	811.07	Joback Method
dvisc	0.0002365	Paxs	579.43	Joback Method

dvisc	0.0002908	Paxs	543.21	Joback Method
dvisc	0.0003681	Paxs	506.98	Joback Method
dvisc	0.0004832	Paxs	470.76	Joback Method
dvisc	0.0006638	Paxs	434.54	Joback Method
dvisc	0.0009661	Paxs	398.31	Joback Method
dvisc	0.0015157	Paxs	362.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1129288&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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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