

3-Bromobenzoic acid, 4-methoxy-2-methylbutyl ester

Inchi:	InChI=1S/C13H17BrO3/c1-10(6-7-16-2)9-17-13(15)11-4-3-5-12(14)8-11/h3-5,8,10H,6-7,9
InchiKey:	ARBAPUNMLUACSR-UHFFFAOYSA-N
Formula:	C13H17BrO3
SMILES:	COCCC(C)COC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	301.18

Physical Properties

Property code	Value	Unit	Source
gf	-165.68	kJ/mol	Joback Method
hf	-442.56	kJ/mol	Joback Method
hfus	28.82	kJ/mol	Joback Method
hvap	65.08	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.279		Crippen Method
mcvol	201.080	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinsol	1974.00		NIST Webbook
tb	692.93	K	Joback Method
tc	909.80	K	Joback Method
tf	414.40	K	Joback Method
vc	0.753	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.91	J/molxK	692.93	Joback Method
cpg	525.19	J/molxK	729.08	Joback Method
cpg	538.55	J/molxK	765.22	Joback Method
cpg	551.00	J/molxK	801.37	Joback Method
cpg	562.57	J/molxK	837.51	Joback Method
cpg	573.27	J/molxK	873.66	Joback Method
cpg	583.12	J/molxK	909.80	Joback Method
dvisc	0.0010442	Paxs	414.40	Joback Method
dvisc	0.0005927	Paxs	460.82	Joback Method

dvisc	0.0003732	Paxs	507.24	Joback Method
dvisc	0.0002539	Paxs	553.67	Joback Method
dvisc	0.0001834	Paxs	600.09	Joback Method
dvisc	0.0001387	Paxs	646.51	Joback Method
dvisc	0.0001090	Paxs	692.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355185&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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