4-Bromobutyric acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C11H13BrO3/c1-14-9-4-6-10(7-5-9)15-11(13)3-2-8-12/h4-7H,2-3,8H2,1H3
InchiKey: RZCZRNVXLRTRTF-UHFFFAOYSA-N
Formula: C11H13BrO3
SMILES: COc1ccc(OC(=O)CCCBr)cc1
Mol. weight [g/mol]: 273.12

Physical Properties

Property code	Value	Unit	Source
gf	-180.08	kJ/mol	Joback Method
hf	-396.00	kJ/mol	Joback Method
hfus	27.16	kJ/mol	Joback Method
hvap	61.02	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.776		Crippen Method
mcvol	172.900	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1821.00		NIST Webbook
rinpol	1821.00		NIST Webbook
tb	647.61	K	Joback Method
tc	867.68	K	Joback Method
tf	406.86	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.94	J/mol×K	647.61	Joback Method
cpg	465.22	J/mol×K	831.00	Joback Method
cpg	455.51	J/mol×K	794.32	Joback Method
cpg	445.04	J/mol×K	757.65	Joback Method
cpg	433.80	J/mol×K	720.97	Joback Method
cpg	421.77	J/mol×K	684.29	Joback Method
cpg	474.17	J/mol×K	867.68	Joback Method
dvisc	0.0001501	Pa×s	647.61	Joback Method

dvisc	0.0001861	Pa×s	607.49	Joback Method
dvisc	0.0002377	Pa×s	567.36	Joback Method
dvisc	0.0003152	Pa×s	527.24	Joback Method
dvisc	0.0004378	Pa×s	487.11	Joback Method
dvisc	0.0006451	Pa×s	446.99	Joback Method
dvisc	0.0010261	Pa×s	406.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307609&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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