5-Bromovaleric acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C12H15BrO3/c1-15-10-5-7-11(8-6-10)16-12(14)4-2-3-9-13/h5-8H,2-4,9H2,1H3
InchiKey: SGXORFYTHBWRII-UHFFFAOYSA-N
Formula: C12H15BrO3
SMILES: COc1ccc(OC(=O)CCCCBr)cc1
Mol. weight [g/mol]: 287.15

Physical Properties

Property code	Value	Unit	Source
gf	-171.66	kJ/mol	Joback Method
hf	-416.64	kJ/mol	Joback Method
hfus	29.75	kJ/mol	Joback Method
hvap	63.25	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.166		Crippen Method
mcvol	186.990	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1951.00		NIST Webbook
rinpol	1951.00		NIST Webbook
tb	670.49	K	Joback Method
tc	886.84	K	Joback Method
tf	418.13	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.95	J/mol×K	670.49	Joback Method
cpg	472.42	J/mol×K	706.55	Joback Method
cpg	485.04	J/mol×K	742.61	Joback Method
cpg	496.84	J/mol×K	778.66	Joback Method
cpg	507.82	J/mol×K	814.72	Joback Method
cpg	518.00	J/mol×K	850.78	Joback Method
cpg	527.40	J/mol×K	886.84	Joback Method
dvisc	0.0009634	Pa×s	418.13	Joback Method

dvisc	0.0005959	Pa×s	460.19	Joback Method
dvisc	0.0003995	Pa×s	502.25	Joback Method
dvisc	0.0002849	Pa×s	544.31	Joback Method
dvisc	0.0002132	Pa×s	586.37	Joback Method
dvisc	0.0001659	Pa×s	628.43	Joback Method
dvisc	0.0001333	Pa×s	670.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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