5-Bromovaleric acid, 3-methylphenyl ester

Inchi: InChI=1S/C12H15BrO2/c1-10-5-4-6-11(9-10)15-12(14)7-2-3-8-13/h4-6,9H,2-3,7-8H2,1H3
InchiKey: ODJQMFULZXKNIQ-UHFFFAOYSA-N
Formula: C12H15BrO2
SMILES: Cc1cccc(OC(=O)CCCCBr)c1
Mol. weight [g/mol]: 271.15

Physical Properties

Property code	Value	Unit	Source
gf	-66.66	kJ/mol	Joback Method
hf	-284.42	kJ/mol	Joback Method
hfus	28.56	kJ/mol	Joback Method
hvap	60.84	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.466		Crippen Method
mcvol	181.120	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	648.07	K	Joback Method
tc	867.01	K	Joback Method
tf	395.90	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.91	J/mol×K	648.07	Joback Method
cpg	447.63	J/mol×K	684.56	Joback Method
cpg	460.50	J/mol×K	721.05	Joback Method
cpg	472.52	J/mol×K	757.54	Joback Method
cpg	483.75	J/mol×K	794.03	Joback Method
cpg	494.20	J/mol×K	830.52	Joback Method
cpg	503.90	J/mol×K	867.01	Joback Method
dvisc	0.0013207	Pa×s	395.90	Joback Method

dvisc	0.0007985	Pa×s	437.93	Joback Method
dvisc	0.0005273	Pa×s	479.96	Joback Method
dvisc	0.0003722	Pa×s	521.99	Joback Method
dvisc	0.0002768	Pa×s	564.01	Joback Method
dvisc	0.0002144	Pa×s	606.04	Joback Method
dvisc	0.0001717	Pa×s	648.07	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=U307641&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