4-Bromobutyric acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C12H15BrO2/c1-9-6-10(2)8-11(7-9)15-12(14)4-3-5-13/h6-8H,3-5H2,1-2H3
InchiKey: AQZLOSMCHRIGGX-UHFFFAOYSA-N
Formula: C12H15BrO2
SMILES: Cc1cc(C)cc(OC(=O)CCCBr)c1
Mol. weight [g/mol]: 271.15

Physical Properties

Property code	Value	Unit	Source
gf	-76.29	kJ/mol	Joback Method
hf	-295.89	kJ/mol	Joback Method
hfus	28.17	kJ/mol	Joback Method
hvap	61.50	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.384		Crippen Method
mcvol	181.120	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	653.05	K	Joback Method
tc	872.87	K	Joback Method
tf	408.42	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.95	J/mol×K	653.05	Joback Method
cpg	446.49	J/mol×K	689.69	Joback Method
cpg	459.21	J/mol×K	726.32	Joback Method
cpg	471.13	J/mol×K	762.96	Joback Method
cpg	482.26	J/mol×K	799.60	Joback Method
cpg	492.64	J/mol×K	836.24	Joback Method
cpg	502.29	J/mol×K	872.87	Joback Method
dvisc	0.0010897	Pa×s	408.42	Joback Method

dvisc	0.0006949	Pa×s	449.19	Joback Method
dvisc	0.0004776	Pa×s	489.96	Joback Method
dvisc	0.0003477	Pa×s	530.74	Joback Method
dvisc	0.0002649	Pa×s	571.51	Joback Method
dvisc	0.0002092	Pa×s	612.28	Joback Method
dvisc	0.0001702	Pa×s	653.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307608&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