4-Bromobutyric acid, 3-methylphenyl ester

Inchi: InChI=1S/C11H13BrO2/c1-9-4-2-5-10(8-9)14-11(13)6-3-7-12/h2,4-5,8H,3,6-7H2,1H3
InchiKey: SXXFVNKMMNIMHS-UHFFFAOYSA-N
Formula: C11H13BrO2
SMILES: Cc1cccc(OC(=O)CCCBr)c1
Mol. weight [g/mol]: 257.12

Physical Properties

Property code	Value	Unit	Source
gf	-75.08	kJ/mol	Joback Method
hf	-263.78	kJ/mol	Joback Method
hfus	25.97	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.076		Crippen Method
mcvol	167.030	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	1664.00		NIST Webbook
rinpol	1664.00		NIST Webbook
tb	625.19	K	Joback Method
tc	848.10	K	Joback Method
tf	384.63	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.72	J/mol×K	625.19	Joback Method
cpg	397.78	J/mol×K	662.34	Joback Method
cpg	410.00	J/mol×K	699.49	Joback Method
cpg	421.43	J/mol×K	736.64	Joback Method
cpg	432.08	J/mol×K	773.79	Joback Method
cpg	441.98	J/mol×K	810.94	Joback Method
cpg	451.17	J/mol×K	848.10	Joback Method
dvisc	0.0013949	Pa×s	384.63	Joback Method

dvisc	0.0008577	Pa×s	424.72	Joback Method
dvisc	0.0005736	Pa×s	464.82	Joback Method
dvisc	0.0004089	Pa×s	504.91	Joback Method
dvisc	0.0003063	Pa×s	545.00	Joback Method
dvisc	0.0002388	Pa×s	585.10	Joback Method
dvisc	0.0001922	Pa×s	625.19	Joback Method

Sources

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=U307606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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