2-Bromopropionic acid, 3-methylphenyl ester

Inchi: InChI=1S/C10H11BrO2/c1-7-4-3-5-9(6-7)13-10(12)8(2)11/h3-6,8H,1-2H3
InchiKey: KWELVYHWGJUSEY-UHFFFAOYSA-N
Formula: C10H11BrO2
SMILES: Cc1cccc(OC(=O)C(C)Br)c1
Mol. weight [g/mol]: 243.10

Physical Properties

Property code	Value	Unit	Source
gf	-85.94	kJ/mol	Joback Method
hf	-248.42	kJ/mol	Joback Method
hfus	19.86	kJ/mol	Joback Method
hvap	56.00	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.684		Crippen Method
mcvol	152.940	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
tb	601.87	K	Joback Method
tc	833.97	K	Joback Method
tf	358.36	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.54	J/mol×K	601.87	Joback Method
cpg	392.43	J/mol×K	795.28	Joback Method
cpg	383.01	J/mol×K	756.60	Joback Method
cpg	372.84	J/mol×K	717.92	Joback Method
cpg	361.89	J/mol×K	679.24	Joback Method
cpg	350.14	J/mol×K	640.55	Joback Method
cpg	401.11	J/mol×K	833.97	Joback Method
dvisc	0.0001996	Pa×s	601.87	Joback Method

dvisc	0.0002516	Pa×s	561.28	Joback Method
dvisc	0.0003287	Pa×s	520.70	Joback Method
dvisc	0.0004493	Pa×s	480.11	Joback Method
dvisc	0.0006506	Pa×s	439.53	Joback Method
dvisc	0.0010158	Pa×s	398.94	Joback Method
dvisc	0.0017544	Pa×s	358.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308023&Units=SI

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