Ethyl 2-(4-bromophenyl)acetate

Other names: Benzeneacetic acid, 4-bromo-, ethyl ester
Ethyl (4-bromophenyl)acetate
4-Bromophenylacetic acid ethyl ester
Inchi: InChI=1S/C10H11BrO2/c1-2-13-10(12)7-8-3-5-9(11)6-4-8/h3-6H,2,7H2,1H3
InchiKey: ZFDCWHPNBWPPHG-UHFFFAOYSA-N
Formula: C10H11BrO2
SMILES: CCOC(=O)Cc1ccc(Br)cc1
Mol. weight [g/mol]: 243.10
CAS: 14062-25-0

Physical Properties

Property code	Value	Unit	Source
gf	-83.50	kJ/mol	Joback Method
hf	-243.14	kJ/mol	Joback Method
hfus	23.38	kJ/mol	Joback Method
hvap	56.38	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.555		Crippen Method
mcvol	152.940	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1583.00		NIST Webbook
tb	602.31	K	Joback Method
tc	829.46	K	Joback Method
tf	373.36	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.08	J/mol×K	602.31	Joback Method
cpg	349.35	J/mol×K	640.17	Joback Method
cpg	360.83	J/mol×K	678.03	Joback Method
cpg	371.55	J/mol×K	715.89	Joback Method
cpg	381.54	J/mol×K	753.74	Joback Method

cpg	390.81	J/mol×K	791.60	Joback Method
cpg	399.40	J/mol×K	829.46	Joback Method
dvisc	0.0014609	Pa×s	373.36	Joback Method
dvisc	0.0009142	Pa×s	411.52	Joback Method
dvisc	0.0006195	Pa×s	449.68	Joback Method
dvisc	0.0004461	Pa×s	487.83	Joback Method
dvisc	0.0003370	Pa×s	525.99	Joback Method
dvisc	0.0002644	Pa×s	564.15	Joback Method
dvisc	0.0002139	Pa×s	602.31	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=C14062250&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