2-Propenoic acid, 3-(4-bromophenyl)-, ethyl ester, (E)-

Other names: Ethyl trans-4-bromocinnamate
Ethyl (2E)-3-(4-bromophenyl)-2-propenoate
trans-p-Bromocinnamic acid ethyl ester
Cinnamic acid, p-bromo-, ethyl ester, (E)-
2-Propenoic acid, 3-(4-bromophenyl)-, ethyl ester

Inchi: InChI=1S/C11H11BrO2/c1-2-14-11(13)8-5-9-3-6-10(12)7-4-9/h3-8H,2H2,1H3/b8-5+

InchiKey: YOOKYIPLSLPRTC-VMPITWQZSA-N

Formula: C11H11BrO2

SMILES: CCOC(=O)C=Cc1ccc(Br)cc1

Mol. weight [g/mol]: 255.11

CAS: 24393-53-1

Physical Properties

Property code	Value	Unit	Source
gf	5.14	kJ/mol	Joback Method
hf	-146.56	kJ/mol	Joback Method
hfus	26.17	kJ/mol	Joback Method
hvap	58.57	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.025		Crippen Method
mcvol	162.730	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	629.35	K	Joback Method
tc	861.83	K	Joback Method
tf	379.55	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.25	J/mol×K	629.35	Joback Method
cpg	375.63	J/mol×K	668.10	Joback Method
cpg	387.15	J/mol×K	706.84	Joback Method
cpg	397.85	J/mol×K	745.59	Joback Method

cpg	407.79	J/mol×K	784.33	Joback Method
cpg	417.00	J/mol×K	823.08	Joback Method
cpg	425.54	J/mol×K	861.83	Joback Method
dvisc	0.0012780	Pa×s	379.55	Joback Method
dvisc	0.0007676	Pa×s	421.18	Joback Method
dvisc	0.0005053	Pa×s	462.82	Joback Method
dvisc	0.0003564	Pa×s	504.45	Joback Method
dvisc	0.0002651	Pa×s	546.08	Joback Method
dvisc	0.0002056	Pa×s	587.72	Joback Method
dvisc	0.0001650	Pa×s	629.35	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.20	K	2.40	NIST Webbook

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=C24393531&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume