Ethyl-«alpha»-bromophenyl acetate

Other names:	Benzeneacetic acid, «alpha»-bromo-, ethyl ester
	Ethyl-alpha-bromophenyl acetate
	ethyl bromophenylacetate
Inchi:	InChI=1S/C10H11BrO2/c1-2-13-10(12)9(11)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3
InchiKey:	BKTKLDMYHTUESO-UHFFFAOYSA-N
Formula:	C10H11BrO2
SMILES:	CCOC(=O)C(Br)c1ccccc1
Mol. weight [g/mol]:	243.10
CAS:	2882-19-1

Physical Properties

Property code	Value	Unit	Source
gf	-76.31	kJ/mol	Joback Method
hf	-236.95	kJ/mol	Joback Method
hfus	20.25	kJ/mol	Joback Method
hvap	55.33	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.686		Crippen Method
mcvol	152.940	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	596.89	K	Joback Method
tc	827.99	K	Joback Method
tf	345.84	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.47	J/mol×K	596.89	Joback Method
cpg	394.19	J/mol×K	789.47	Joback Method
cpg	384.68	J/mol×K	750.96	Joback Method
cpg	374.39	J/mol×K	712.44	Joback Method
cpg	363.29	J/mol×K	673.92	Joback Method
cpg	351.33	J/mol×K	635.41	Joback Method

cpg	402.94	J/mol×K	827.99	Joback Method
dvisc	0.0002034	Pa×s	596.89	Joback Method
dvisc	0.0002610	Pa×s	555.05	Joback Method
dvisc	0.0003490	Pa×s	513.21	Joback Method
dvisc	0.0004912	Pa×s	471.37	Joback Method
dvisc	0.0007389	Pa×s	429.52	Joback Method
dvisc	0.0012142	Pa×s	387.68	Joback Method
dvisc	0.0022498	Pa×s	345.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.00 ± 1.00	K	2.40	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2882191&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
tb: Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume