2(P-bromophenoxy)ethyl alpha,alpha-dichloropropionate

Inchi: InChI=1S/C11H11BrCl2O3/c1-11(13,14)10(15)17-7-6-16-9-4-2-8(12)3-5-9/h2-5H,6-7H2,1

InchiKey: KQILBCATKAJIDX-UHFFFAOYSA-N

Formula: C11H11BrCl2O3

SMILES: CC(Cl)(Cl)C(=O)OCCOc1ccc(Br)cc1

Mol. weight [g/mol]: 342.01

CAS: 99852-98-9

Physical Properties

Property code	Value	Unit	Source
gf	-201.10	kJ/mol	Joback Method
hf	-436.23	kJ/mol	Joback Method
hfus	28.14	kJ/mol	Joback Method
hvap	68.49	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.565		Crippen Method
mcvol	197.380	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
tb	719.24	K	Joback Method
tc	957.76	K	Joback Method
tf	469.12	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.29	J/mol×K	719.24	Joback Method
cpg	469.39	J/mol×K	758.99	Joback Method
cpg	479.55	J/mol×K	798.75	Joback Method
cpg	488.83	J/mol×K	838.50	Joback Method
cpg	497.26	J/mol×K	878.25	Joback Method
cpg	504.90	J/mol×K	918.00	Joback Method
cpg	511.80	J/mol×K	957.76	Joback Method
dvisc	0.0007303	Pa×s	469.12	Joback Method
dvisc	0.0004576	Pa×s	510.81	Joback Method

dvisc	0.0003077	Pa×s	552.49	Joback Method
dvisc	0.0002188	Pa×s	594.18	Joback Method
dvisc	0.0001627	Pa×s	635.87	Joback Method
dvisc	0.0001254	Pa×s	677.55	Joback Method
dvisc	0.0000997	Pa×s	719.24	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=C99852989&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume