2,4-Dibromophenyl propionate

Inchi: InChI=1S/C9H8Br2O2/c1-2-9(12)13-8-4-3-6(10)5-7(8)11/h3-5H,2H2,1H3
InchiKey: ISVXJOYTEWPLSM-UHFFFAOYSA-N
Formula: C9H8Br2O2
SMILES: CCC(=O)Oc1ccc(Br)cc1Br
Mol. weight [g/mol]: 307.97
CAS: 23689-34-1

Physical Properties

Property code	Value	Unit	Source
gf	-87.23	kJ/mol	Joback Method
hf	-207.64	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	61.25	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.527		Crippen Method
mcvol	156.350	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	650.57	K	Joback Method
tc	895.55	K	Joback Method
tf	434.41	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.76	J/mol×K	650.57	Joback Method
cpg	330.72	J/mol×K	691.40	Joback Method
cpg	339.96	J/mol×K	732.23	Joback Method
cpg	348.51	J/mol×K	773.06	Joback Method
cpg	356.38	J/mol×K	813.89	Joback Method
cpg	363.62	J/mol×K	854.72	Joback Method
cpg	370.26	J/mol×K	895.55	Joback Method
dvisc	0.0010010	Pa×s	434.41	Joback Method
dvisc	0.0007003	Pa×s	470.44	Joback Method

dvisc	0.0005154	Pa×s	506.46	Joback Method
dvisc	0.0003952	Pa×s	542.49	Joback Method
dvisc	0.0003131	Pa×s	578.52	Joback Method
dvisc	0.0002550	Pa×s	614.54	Joback Method
dvisc	0.0002124	Pa×s	650.57	Joback Method

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=C23689341&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume