Diglycolic acid, 4-bromophenyl ethyl ester

Inchi: InChI=1S/C12H13BrO5/c1-2-17-11(14)7-16-8-12(15)18-10-5-3-9(13)4-6-10/h3-6H,2,7-8H
InchiKey: ZHPIODIONHJSLY-UHFFFAOYSA-N
Formula: C12H13BrO5
SMILES: CCOC(=O)COCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 317.13

Physical Properties

Property code	Value	Unit	Source
gf	-405.58	kJ/mol	Joback Method
hf	-661.44	kJ/mol	Joback Method
hfus	32.53	kJ/mol	Joback Method
hvap	72.40	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.934		Crippen Method
mcvol	194.430	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	2513.00		NIST Webbook
tb	746.78	K	Joback Method
tc	966.76	K	Joback Method
tf	490.29	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.94	J/mol×K	746.78	Joback Method
cpg	546.53	J/mol×K	930.10	Joback Method
cpg	538.42	J/mol×K	893.44	Joback Method
cpg	529.40	J/mol×K	856.77	Joback Method
cpg	519.48	J/mol×K	820.11	Joback Method
cpg	508.66	J/mol×K	783.44	Joback Method
cpg	553.73	J/mol×K	966.76	Joback Method
dvisc	0.0001008	Pa×s	746.78	Joback Method
dvisc	0.0001241	Pa×s	704.03	Joback Method

dvisc	0.0001571	Pa×s	661.28	Joback Method
dvisc	0.0002055	Pa×s	618.54	Joback Method
dvisc	0.0002796	Pa×s	575.79	Joback Method
dvisc	0.0003997	Pa×s	533.04	Joback Method
dvisc	0.0006081	Pa×s	490.29	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=U381892&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