Diethylmalonic acid, 4-bromophenyl isobutyl ester

Inchi: InChI=1S/C17H23BrO4/c1-5-17(6-2,15(19)21-11-12(3)4)16(20)22-14-9-7-13(18)8-10-14/

InchiKey: IJFDBOMRTMERGR-UHFFFAOYSA-N

Formula: C17H23BrO4

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 371.27

Physical Properties

Property code	Value	Unit	Source
gf	-258.08	kJ/mol	Joback Method
hf	-646.45	kJ/mol	Joback Method
hfus	33.36	kJ/mol	Joback Method
hvap	79.44	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.360		Crippen Method
mcvol	259.010	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
tb	835.09	K	Joback Method
tc	1056.32	K	Joback Method
tf	511.83	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.93	J/mol×K	835.09	Joback Method
cpg	760.08	J/mol×K	871.96	Joback Method
cpg	773.12	J/mol×K	908.83	Joback Method
cpg	785.10	J/mol×K	945.71	Joback Method
cpg	796.08	J/mol×K	982.58	Joback Method
cpg	806.09	J/mol×K	1019.45	Joback Method
cpg	815.20	J/mol×K	1056.32	Joback Method
dvisc	0.0005423	Pa×s	511.83	Joback Method

dvisc	0.0002994	Pa×s	565.71	Joback Method
dvisc	0.0001833	Pa×s	619.58	Joback Method
dvisc	0.0001213	Pa×s	673.46	Joback Method
dvisc	0.0000854	Pa×s	727.34	Joback Method
dvisc	0.0000631	Pa×s	781.21	Joback Method
dvisc	0.0000485	Pa×s	835.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369822&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

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