Diethylmalonic acid, 4-bromophenyl ethyl ester

Inchi: InChI=1S/C15H19BrO4/c1-4-15(5-2,13(17)19-6-3)14(18)20-12-9-7-11(16)8-10-12/h7-10H

InchiKey: RTMGFWQMWDZZCG-UHFFFAOYSA-N

Formula: C15H19BrO4

SMILES: CCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 343.21

Physical Properties

Property code	Value	Unit	Source
gf	-272.48	kJ/mol	Joback Method
hf	-599.89	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	75.37	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.724		Crippen Method
mcvol	230.830	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	2018.00		NIST Webbook
rinpol	2018.00		NIST Webbook
tb	789.77	K	Joback Method
tc	1012.85	K	Joback Method
tf	504.29	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.08	J/mol×K	789.77	Joback Method
cpg	691.42	J/mol×K	975.67	Joback Method
cpg	681.86	J/mol×K	938.49	Joback Method
cpg	671.39	J/mol×K	901.31	Joback Method
cpg	659.97	J/mol×K	864.13	Joback Method
cpg	647.55	J/mol×K	826.95	Joback Method
cpg	700.11	J/mol×K	1012.85	Joback Method
dvisc	0.0000713	Pa×s	789.77	Joback Method

dvisc	0.0000908	Pa×s	742.19	Joback Method
dvisc	0.0001194	Pa×s	694.61	Joback Method
dvisc	0.0001634	Pa×s	647.03	Joback Method
dvisc	0.0002351	Pa×s	599.45	Joback Method
dvisc	0.0003603	Pa×s	551.87	Joback Method
dvisc	0.0005983	Pa×s	504.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369821&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume