Diethylmalonic acid, 4-bromo-2-methoxyphenyl propyl ester

Inchi: InChI=1S/C17H23BrO5/c1-5-10-22-15(19)17(6-2,7-3)16(20)23-13-9-8-12(18)11-14(13)21

InchiKey: ZAIATAUBFHHZTP-UHFFFAOYSA-N

Formula: C17H23BrO5

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 387.27

Physical Properties

Property code	Value	Unit	Source
gf	-370.27	kJ/mol	Joback Method
hf	-784.86	kJ/mol	Joback Method
hfus	37.68	kJ/mol	Joback Method
hvap	82.90	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.123		Crippen Method
mcvol	264.880	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	2274.00		NIST Webbook
tb	862.93	K	Joback Method
tc	1081.17	K	Joback Method
tf	561.58	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.29	J/mol×K	862.93	Joback Method
cpg	827.08	J/mol×K	1044.79	Joback Method
cpg	818.08	J/mol×K	1008.42	Joback Method
cpg	808.02	J/mol×K	972.05	Joback Method
cpg	796.89	J/mol×K	935.68	Joback Method
cpg	784.66	J/mol×K	899.30	Joback Method
cpg	835.05	J/mol×K	1081.17	Joback Method
dvisc	0.0000397	Pa×s	862.93	Joback Method
dvisc	0.0000500	Pa×s	812.70	Joback Method

dvisc	0.0000649	Pa×s	762.48	Joback Method
dvisc	0.0000874	Pa×s	712.25	Joback Method
dvisc	0.0001233	Pa×s	662.03	Joback Method
dvisc	0.0001839	Pa×s	611.81	Joback Method
dvisc	0.0002948	Pa×s	561.58	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=U370938&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume