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

Inchi: InChI=1S/C16H21BrO5/c1-5-16(6-2,14(18)21-7-3)15(19)22-12-9-8-11(17)10-13(12)20-4/

InchiKey: WJRNSZVOAVWJBH-UHFFFAOYSA-N

Formula: C16H21BrO5

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

Mol. weight [g/mol]: 373.24

Physical Properties

Property code	Value	Unit	Source
gf	-378.69	kJ/mol	Joback Method
hf	-764.22	kJ/mol	Joback Method
hfus	35.09	kJ/mol	Joback Method
hvap	80.67	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.733		Crippen Method
mcvol	250.790	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	2193.00		NIST Webbook
tb	840.05	K	Joback Method
tc	1059.83	K	Joback Method
tf	550.31	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.73	J/mol×K	840.05	Joback Method
cpg	727.90	J/mol×K	876.68	Joback Method
cpg	739.96	J/mol×K	913.31	Joback Method
cpg	750.94	J/mol×K	949.94	Joback Method
cpg	760.87	J/mol×K	986.57	Joback Method
cpg	769.77	J/mol×K	1023.20	Joback Method
cpg	777.66	J/mol×K	1059.83	Joback Method
dvisc	0.0003286	Pa×s	550.31	Joback Method
dvisc	0.0002076	Pa×s	598.60	Joback Method

dvisc	0.0001405	Pa×s	646.89	Joback Method
dvisc	0.0001004	Pa×s	695.18	Joback Method
dvisc	0.0000749	Pa×s	743.47	Joback Method
dvisc	0.0000579	Pa×s	791.76	Joback Method
dvisc	0.0000462	Pa×s	840.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370935&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