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

Inchi: InChI=1S/C18H25BrO5/c1-6-18(7-2,16(20)23-11-12(3)4)17(21)24-14-9-8-13(19)10-15(14

InchiKey: DGWIJMXIPRGFQK-UHFFFAOYSA-N

Formula: C18H25BrO5

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 401.29

Physical Properties

Property code	Value	Unit	Source
gf	-364.29	kJ/mol	Joback Method
hf	-810.78	kJ/mol	Joback Method
hfus	36.75	kJ/mol	Joback Method
hvap	84.73	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.369		Crippen Method
mcvol	278.970	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2317.00		NIST Webbook
tb	885.37	K	Joback Method
tc	1105.08	K	Joback Method
tf	557.85	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.20	J/mol×K	885.37	Joback Method
cpg	842.85	J/mol×K	921.99	Joback Method
cpg	855.30	J/mol×K	958.61	Joback Method
cpg	866.59	J/mol×K	995.23	Joback Method
cpg	876.73	J/mol×K	1031.84	Joback Method
cpg	885.77	J/mol×K	1068.46	Joback Method
cpg	893.72	J/mol×K	1105.08	Joback Method
dvisc	0.0002882	Pa×s	557.85	Joback Method
dvisc	0.0001686	Pa×s	612.44	Joback Method

dvisc	0.0001076	Pa×s	667.02	Joback Method
dvisc	0.0000735	Pa×s	721.61	Joback Method
dvisc	0.0000530	Pa×s	776.20	Joback Method
dvisc	0.0000399	Pa×s	830.78	Joback Method
dvisc	0.0000311	Pa×s	885.37	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=U370939&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