Diethylmalonic acid, di(4-bromo-2-methoxyphenyl) ester

Inchi: InChI=1S/C21H22Br2O6/c1-5-21(6-2,19(24)28-15-9-7-13(22)11-17(15)26-3)20(25)29-16
InchiKey: IICCVYBQMZFDFT-UHFFFAOYSA-N
Formula: C21H22Br2O6
SMILES: CCC(CC)(C(=O)Oc1ccc(Br)cc1OC)C(=O)Oc1ccc(Br)cc1OC
Mol. weight [g/mol]: 530.20

Physical Properties

Property code	Value	Unit	Source
gf	-334.12	kJ/mol	Joback Method
hf	-759.72	kJ/mol	Joback Method
hfus	47.78	kJ/mol	Joback Method
hvap	104.25	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	5.546		Crippen Method
mcvol	320.850	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	3201.00		NIST Webbook
rinpol	3201.00		NIST Webbook
tb	1079.67	K	Joback Method
tc	1331.43	K	Joback Method
tf	740.15	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.81	J/mol×K	1079.67	Joback Method
cpg	970.24	J/mol×K	1289.47	Joback Method
cpg	968.04	J/mol×K	1247.51	Joback Method
cpg	964.44	J/mol×K	1205.55	Joback Method
cpg	959.40	J/mol×K	1163.59	Joback Method
cpg	952.87	J/mol×K	1121.63	Joback Method
cpg	971.07	J/mol×K	1331.43	Joback Method
dvisc	0.0000123	Pa×s	1079.67	Joback Method

dvisc	0.0000150	Pa×s	1023.08	Joback Method
dvisc	0.0000189	Pa×s	966.50	Joback Method
dvisc	0.0000243	Pa×s	909.91	Joback Method
dvisc	0.0000324	Pa×s	853.32	Joback Method
dvisc	0.0000449	Pa×s	796.74	Joback Method
dvisc	0.0000656	Pa×s	740.15	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=U371165&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