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

Inchi: InChI=1S/C26H41BrO5/c1-5-8-9-10-11-12-13-14-15-16-19-31-24(28)26(6-2,7-3)25(29)32

InchiKey: WTUGAVFRFVSRRG-UHFFFAOYSA-N

Formula: C26H41BrO5

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

Mol. weight [g/mol]: 513.50

Physical Properties

Property code	Value	Unit	Source
gf	-294.49	kJ/mol	Joback Method
hf	-970.62	kJ/mol	Joback Method
hfus	60.99	kJ/mol	Joback Method
hvap	102.93	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	7.634		Crippen Method
mcvol	391.690	ml/mol	McGowan Method
pc	946.75	kPa	Joback Method
rinpol	3130.00		NIST Webbook
tb	1068.85	K	Joback Method
tc	1310.37	K	Joback Method
tf	663.01	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1309.59	J/mol×K	1068.85	Joback Method
cpg	1368.36	J/mol×K	1270.12	Joback Method
cpg	1359.56	J/mol×K	1229.87	Joback Method
cpg	1349.36	J/mol×K	1189.61	Joback Method
cpg	1337.69	J/mol×K	1149.36	Joback Method
cpg	1324.45	J/mol×K	1109.10	Joback Method
cpg	1375.83	J/mol×K	1310.37	Joback Method
dvisc	0.0000094	Pa×s	1068.85	Joback Method
dvisc	0.0000122	Pa×s	1001.21	Joback Method

dvisc	0.0000164	Pa×s	933.57	Joback Method
dvisc	0.0000230	Pa×s	865.93	Joback Method
dvisc	0.0000343	Pa×s	798.29	Joback Method
dvisc	0.0000550	Pa×s	730.65	Joback Method
dvisc	0.0000972	Pa×s	663.01	Joback Method

Sources

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=U371163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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