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

Inchi: InChI=1S/C23H35BrO5/c1-5-8-9-10-11-12-13-16-28-21(25)23(6-2,7-3)22(26)29-19-15-14

InchiKey: NIPXWOGZCVTIDX-UHFFFAOYSA-N

Formula: C23H35BrO5

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

Mol. weight [g/mol]: 471.43

Physical Properties

Property code	Value	Unit	Source
gf	-319.75	kJ/mol	Joback Method
hf	-908.70	kJ/mol	Joback Method
hfus	53.22	kJ/mol	Joback Method
hvap	96.25	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	6.463		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	2822.00		NIST Webbook
tb	1000.21	K	Joback Method
tc	1225.35	K	Joback Method
tf	629.20	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.47	J/mol×K	1000.21	Joback Method
cpg	1183.50	J/mol×K	1187.82	Joback Method
cpg	1174.47	J/mol×K	1150.30	Joback Method
cpg	1164.21	J/mol×K	1112.78	Joback Method
cpg	1152.65	J/mol×K	1075.26	Joback Method
cpg	1139.76	J/mol×K	1037.73	Joback Method
cpg	1191.35	J/mol×K	1225.35	Joback Method
dvisc	0.0000154	Pa×s	1000.21	Joback Method
dvisc	0.0000198	Pa×s	938.38	Joback Method

dvisc	0.0000263	Pa×s	876.54	Joback Method
dvisc	0.0000365	Pa×s	814.71	Joback Method
dvisc	0.0000535	Pa×s	752.87	Joback Method
dvisc	0.0000840	Pa×s	691.04	Joback Method
dvisc	0.0001439	Pa×s	629.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370905&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