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

Inchi: InChI=1S/C28H45BrO5/c1-5-8-9-10-11-12-13-14-15-16-17-18-21-33-26(30)28(6-2,7-3)27

InchiKey: KZUJTJXKNPIKII-UHFFFAOYSA-N

Formula: C28H45BrO5

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

Mol. weight [g/mol]: 541.56

Physical Properties

Property code	Value	Unit	Source
gf	-277.65	kJ/mol	Joback Method
hf	-1011.90	kJ/mol	Joback Method
hfus	66.17	kJ/mol	Joback Method
hvap	107.38	kJ/mol	Joback Method
log10ws	-9.64		Crippen Method
logp	8.414		Crippen Method
mcvol	419.870	ml/mol	McGowan Method
pc	844.07	kPa	Joback Method
rinpol	3326.00		NIST Webbook
rinpol	3326.00		NIST Webbook
tb	1114.61	K	Joback Method
tc	1373.14	K	Joback Method
tf	685.55	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1434.10	J/mol×K	1114.61	Joback Method
cpg	1449.48	J/mol×K	1157.70	Joback Method
cpg	1463.00	J/mol×K	1200.79	Joback Method
cpg	1474.76	J/mol×K	1243.88	Joback Method
cpg	1484.88	J/mol×K	1286.96	Joback Method
cpg	1493.45	J/mol×K	1330.05	Joback Method
cpg	1500.59	J/mol×K	1373.14	Joback Method
dvisc	0.0000740	Pa×s	685.55	Joback Method

dvisc	0.0000412	Pa×s	757.06	Joback Method
dvisc	0.0000253	Pa×s	828.57	Joback Method
dvisc	0.0000168	Pa×s	900.08	Joback Method
dvisc	0.0000119	Pa×s	971.59	Joback Method
dvisc	0.0000088	Pa×s	1043.10	Joback Method
dvisc	0.0000068	Pa×s	1114.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U371164&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