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

Inchi: InChI=1S/C24H37BrO5/c1-5-8-9-10-11-12-13-14-17-29-22(26)24(6-2,7-3)23(27)30-20-16

InchiKey: UALFWWVKQMBOCH-UHFFFAOYSA-N

Formula: C24H37BrO5

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

Mol. weight [g/mol]: 485.45

Physical Properties

Property code	Value	Unit	Source
gf	-311.33	kJ/mol	Joback Method
hf	-929.34	kJ/mol	Joback Method
hfus	55.81	kJ/mol	Joback Method
hvap	98.48	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	6.853		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
pc	1069.36	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	1023.09	K	Joback Method
tc	1252.58	K	Joback Method
tf	640.47	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.44	J/mol×K	1023.09	Joback Method
cpg	1244.71	J/mol×K	1214.33	Joback Method
cpg	1235.74	J/mol×K	1176.08	Joback Method
cpg	1225.49	J/mol×K	1137.83	Joback Method
cpg	1213.89	J/mol×K	1099.59	Joback Method
cpg	1200.90	J/mol×K	1061.34	Joback Method
cpg	1252.45	J/mol×K	1252.58	Joback Method
dvisc	0.0000131	Pa×s	1023.09	Joback Method

dvisc	0.0000169	Pa×s	959.32	Joback Method
dvisc	0.0000225	Pa×s	895.55	Joback Method
dvisc	0.0000314	Pa×s	831.78	Joback Method
dvisc	0.0000462	Pa×s	768.01	Joback Method
dvisc	0.0000731	Pa×s	704.24	Joback Method
dvisc	0.0001266	Pa×s	640.47	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=U371161&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