2,6-Naphthalenedicarboxylic acid, 3-[4-[decahydro-5-hydroxy-1-(methoxycarbonyl)-1 dimethyl ester

Inchi: InChI=1S/C33H44O8/c1-19-16-25-21(18-24(19)30(35)39-4)17-20(28(29(25)38-3)31(36)4

InchiKey: ZHBUKQIDKMXZAI-UHFFFAOYSA-N

Formula: C33H44O8

SMILES: COC(=O)c1cc2cc(CCCCC3CCC4C(O)CCCC4C3(C)C(=O)OC)c(C(=O)OC)c(OC)c2cc1C

Mol. weight [g/mol]: 568.70

CAS: 56704-52-0

Physical Properties

Property code	Value	Unit	Source
gf	-501.21	kJ/mol	Joback Method
hf	-1297.87	kJ/mol	Joback Method
hfus	68.76	kJ/mol	Joback Method
hvap	141.27	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	5.809		Crippen Method
mcvol	444.950	ml/mol	McGowan Method
pc	882.62	kPa	Joback Method
tb	1385.26	K	Joback Method
tc	1751.32	K	Joback Method
tf	915.90	K	Joback Method
vc	1.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1762.74	J/mol×K	1385.26	Joback Method
cpg	1792.24	J/mol×K	1446.27	Joback Method
cpg	1822.21	J/mol×K	1507.28	Joback Method
cpg	1853.25	J/mol×K	1568.29	Joback Method
cpg	1885.90	J/mol×K	1629.30	Joback Method
cpg	1920.75	J/mol×K	1690.31	Joback Method
cpg	1958.36	J/mol×K	1751.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56704520&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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume