Delta 1(2)-alpha- naphthalenemalonic acid, 3-hydroxy-4-oxo-, diethyl ester

Inchi: InChI=1S/C17H16O6/c1-3-22-16(20)14(17(21)23-4-2)12-9-13(18)15(19)11-8-6-5-7-10(11

InchiKey: NOYJQYUJKVGDGF-UHFFFAOYSA-N

Formula: C17H16O6

SMILES: CCOC(=O)C(C(=O)OCC)=C1C=C(O)C(=O)c2ccccc21

Mol. weight [g/mol]: 316.31

CAS: 7475-39-0

Physical Properties

Property code	Value	Unit	Source
gf	-418.61	kJ/mol	Joback Method
hf	-749.15	kJ/mol	Joback Method
hfus	37.42	kJ/mol	Joback Method
hvap	97.83	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.205		Crippen Method
mcvol	229.490	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
tb	958.94	K	Joback Method
tc	1186.99	K	Joback Method
tf	621.99	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.60	J/mol×K	958.94	Joback Method
cpg	713.19	J/mol×K	996.95	Joback Method
cpg	721.65	J/mol×K	1034.96	Joback Method
cpg	728.98	J/mol×K	1072.96	Joback Method
cpg	735.22	J/mol×K	1110.97	Joback Method
cpg	740.36	J/mol×K	1148.98	Joback Method
cpg	744.42	J/mol×K	1186.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7475390&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
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