Diethylmalonic acid, 2-formylphenyl hexadecyl ester

Inchi: InChI=1S/C30H48O5/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-21-24-34-28(32)30(5-2,6-3
InchiKey: WBPBOWQFKCMJAJ-UHFFFAOYSA-N
Formula: C30H48O5
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 488.70

Physical Properties

Property code	Value	Unit	Source
gf	-260.02	kJ/mol	Joback Method
hf	-1021.40	kJ/mol	Joback Method
hfus	67.56	kJ/mol	Joback Method
hvap	109.05	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	8.235		Crippen Method
mcvol	426.250	ml/mol	McGowan Method
pc	772.89	kPa	Joback Method
rinpol	3376.00		NIST Webbook
tb	1115.47	K	Joback Method
tc	1381.46	K	Joback Method
tf	655.54	K	Joback Method
vc	1.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1507.80	J/mol×K	1115.47	Joback Method
cpg	1525.16	J/mol×K	1159.80	Joback Method
cpg	1540.65	J/mol×K	1204.13	Joback Method
cpg	1554.42	J/mol×K	1248.47	Joback Method
cpg	1566.64	J/mol×K	1292.80	Joback Method
cpg	1577.45	J/mol×K	1337.13	Joback Method
cpg	1587.00	J/mol×K	1381.46	Joback Method
dvisc	0.0001402	Pa×s	655.54	Joback Method
dvisc	0.0000707	Pa×s	732.19	Joback Method

dvisc	0.0000406	Pa×s	808.85	Joback Method
dvisc	0.0000257	Pa×s	885.50	Joback Method
dvisc	0.0000174	Pa×s	962.16	Joback Method
dvisc	0.0000126	Pa×s	1038.81	Joback Method
dvisc	0.0000095	Pa×s	1115.47	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=U369961&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