Diethylmalonic acid, 2-formylphenyl undecyl ester

Inchi: InChI=1S/C25H38O5/c1-4-7-8-9-10-11-12-13-16-19-29-23(27)25(5-2,6-3)24(28)30-22-18
InchiKey: BQGNCUHHIWQQDJ-UHFFFAOYSA-N
Formula: C25H38O5
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 418.57

Physical Properties

Property code	Value	Unit	Source
gf	-302.12	kJ/mol	Joback Method
hf	-918.20	kJ/mol	Joback Method
hfus	54.61	kJ/mol	Joback Method
hvap	97.92	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.285		Crippen Method
mcvol	355.800	ml/mol	McGowan Method
pc	1029.26	kPa	Joback Method
rinpol	2850.00		NIST Webbook
tb	1001.07	K	Joback Method
tc	1225.60	K	Joback Method
tf	599.19	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.29	J/mol×K	1001.07	Joback Method
cpg	1210.77	J/mol×K	1038.49	Joback Method
cpg	1224.87	J/mol×K	1075.91	Joback Method
cpg	1237.67	J/mol×K	1113.33	Joback Method
cpg	1249.23	J/mol×K	1150.76	Joback Method
cpg	1259.63	J/mol×K	1188.18	Joback Method
cpg	1268.94	J/mol×K	1225.60	Joback Method
dvisc	0.0002738	Pa×s	599.19	Joback Method
dvisc	0.0001443	Pa×s	666.17	Joback Method

dvisc	0.0000855	Pa×s	733.15	Joback Method
dvisc	0.0000553	Pa×s	800.13	Joback Method
dvisc	0.0000383	Pa×s	867.11	Joback Method
dvisc	0.0000279	Pa×s	934.09	Joback Method
dvisc	0.0000212	Pa×s	1001.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369956&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
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