Diethylmalonic acid, dodecyl 2-formylphenyl ester

Inchi: InChI=1S/C26H40O5/c1-4-7-8-9-10-11-12-13-14-17-20-30-24(28)26(5-2,6-3)25(29)31-23

InchiKey: ZDRIZTCWPOFZKI-UHFFFAOYSA-N

Formula: C26H40O5

SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C=O

Mol. weight [g/mol]: 432.59

Physical Properties

Property code	Value	Unit	Source
gf	-293.70	kJ/mol	Joback Method
hf	-938.84	kJ/mol	Joback Method
hfus	57.20	kJ/mol	Joback Method
hvap	100.14	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.675		Crippen Method
mcvol	369.890	ml/mol	McGowan Method
pc	968.68	kPa	Joback Method
rinpol	2964.00		NIST Webbook
tb	1023.95	K	Joback Method
tc	1254.29	K	Joback Method
tf	610.46	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.02	J/mol×K	1023.95	Joback Method
cpg	1322.19	J/mol×K	1215.90	Joback Method
cpg	1311.74	J/mol×K	1177.51	Joback Method
cpg	1300.07	J/mol×K	1139.12	Joback Method
cpg	1287.12	J/mol×K	1100.73	Joback Method
cpg	1272.80	J/mol×K	1062.34	Joback Method
cpg	1331.53	J/mol×K	1254.29	Joback Method
dvisc	0.0000181	Pa×s	1023.95	Joback Method
dvisc	0.0000239	Pa×s	955.03	Joback Method

dvisc	0.0000328	Pa×s	886.12	Joback Method
dvisc	0.0000476	Pa×s	817.20	Joback Method
dvisc	0.0000739	Pa×s	748.29	Joback Method
dvisc	0.0001256	Pa×s	679.38	Joback Method
dvisc	0.0002406	Pa×s	610.46	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369957&Units=SI

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