Diethylmalonic acid, 2-formylphenyl pentyl ester

Inchi: InChI=1S/C19H26O5/c1-4-7-10-13-23-17(21)19(5-2,6-3)18(22)24-16-12-9-8-11-15(16)14

InchiKey: IUQMZKXEXKXJFG-UHFFFAOYSA-N

Formula: C19H26O5

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

Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-352.64	kJ/mol	Joback Method
hf	-794.36	kJ/mol	Joback Method
hfus	39.07	kJ/mol	Joback Method
hvap	84.56	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.944		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2251.00		NIST Webbook
tb	863.79	K	Joback Method
tc	1073.78	K	Joback Method
tf	531.57	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.13	J/mol×K	863.79	Joback Method
cpg	896.40	J/mol×K	1038.78	Joback Method
cpg	886.41	J/mol×K	1003.78	Joback Method
cpg	875.43	J/mol×K	968.78	Joback Method
cpg	863.42	J/mol×K	933.79	Joback Method
cpg	850.33	J/mol×K	898.79	Joback Method
cpg	905.44	J/mol×K	1073.78	Joback Method
dvisc	0.0000534	Pa×s	863.79	Joback Method
dvisc	0.0000690	Pa×s	808.42	Joback Method

dvisc	0.0000928	Pa×s	753.05	Joback Method
dvisc	0.0001307	Pa×s	697.68	Joback Method
dvisc	0.0001954	Pa×s	642.31	Joback Method
dvisc	0.0003149	Pa×s	586.94	Joback Method
dvisc	0.0005608	Pa×s	531.57	Joback Method

Sources

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=U369950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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