Diethylmalonic acid, di(2-formylphenyl) ester

Inchi: InChI=1S/C21H20O6/c1-3-21(4-2,19(24)26-17-11-7-5-9-15(17)13-22)20(25)27-18-12-8-6
InchiKey: RRAMFOAYFMRLNN-UHFFFAOYSA-N
Formula: C21H20O6
SMILES: CCC(CC)(C(=O)Oc1ccccc1C=O)C(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 368.38

Physical Properties

Property code	Value	Unit	Source
gf	-332.54	kJ/mol	Joback Method
hf	-696.16	kJ/mol	Joback Method
hfus	40.19	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	3.629		Crippen Method
mcvol	277.250	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2800.00		NIST Webbook
tb	989.87	K	Joback Method
tc	1227.39	K	Joback Method
tf	635.05	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.96	J/mol×K	989.87	Joback Method
cpg	865.09	J/mol×K	1029.46	Joback Method
cpg	873.99	J/mol×K	1069.04	Joback Method
cpg	881.75	J/mol×K	1108.63	Joback Method
cpg	888.41	J/mol×K	1148.22	Joback Method
cpg	894.06	J/mol×K	1187.80	Joback Method
cpg	898.75	J/mol×K	1227.39	Joback Method
dvisc	0.0003367	Pa×s	635.05	Joback Method
dvisc	0.0002074	Pa×s	694.19	Joback Method

dvisc	0.0001378	Pa×s	753.32	Joback Method
dvisc	0.0000972	Pa×s	812.46	Joback Method
dvisc	0.0000719	Pa×s	871.60	Joback Method
dvisc	0.0000552	Pa×s	930.73	Joback Method
dvisc	0.0000438	Pa×s	989.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369962&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
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