Diethylmalonic acid, 2-formylphenyl isobutyl ester

Inchi: InChI=1S/C18H24O5/c1-5-18(6-2,16(20)22-12-13(3)4)17(21)23-15-10-8-7-9-14(15)11-19

InchiKey: PFLOSFYWGHNDIQ-UHFFFAOYSA-N

Formula: C18H24O5

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1ccccc1C=O

Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-363.50	kJ/mol	Joback Method
hf	-779.00	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	81.95	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.410		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
tb	840.47	K	Joback Method
tc	1053.32	K	Joback Method
tf	505.30	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.20	J/mol×K	840.47	Joback Method
cpg	793.34	J/mol×K	875.94	Joback Method
cpg	806.36	J/mol×K	911.42	Joback Method
cpg	818.30	J/mol×K	946.89	Joback Method
cpg	829.19	J/mol×K	982.37	Joback Method
cpg	839.07	J/mol×K	1017.84	Joback Method
cpg	847.98	J/mol×K	1053.32	Joback Method
dvisc	0.0007049	Pa×s	505.30	Joback Method

dvisc	0.0003756	Pa×s	561.16	Joback Method
dvisc	0.0002243	Pa×s	617.02	Joback Method
dvisc	0.0001460	Pa×s	672.88	Joback Method
dvisc	0.0001014	Pa×s	728.75	Joback Method
dvisc	0.0000742	Pa×s	784.61	Joback Method
dvisc	0.0000566	Pa×s	840.47	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=U369948&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