Diethylmalonic acid, 2-formylphenyl nonyl ester

Inchi: InChI=1S/C23H34O5/c1-4-7-8-9-10-11-14-17-27-21(25)23(5-2,6-3)22(26)28-20-16-13-12

InchiKey: GGCKWLGTWBMEQR-UHFFFAOYSA-N

Formula: C23H34O5

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

Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-318.96	kJ/mol	Joback Method
hf	-876.92	kJ/mol	Joback Method
hfus	49.43	kJ/mol	Joback Method
hvap	93.47	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.505		Crippen Method
mcvol	327.620	ml/mol	McGowan Method
pc	1168.82	kPa	Joback Method
rinpol	2650.00		NIST Webbook
tb	955.31	K	Joback Method
tc	1171.38	K	Joback Method
tf	576.65	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.23	J/mol×K	955.31	Joback Method
cpg	1136.14	J/mol×K	1135.37	Joback Method
cpg	1125.85	J/mol×K	1099.36	Joback Method
cpg	1114.47	J/mol×K	1063.35	Joback Method
cpg	1101.95	J/mol×K	1027.33	Joback Method
cpg	1088.22	J/mol×K	991.32	Joback Method
cpg	1145.39	J/mol×K	1171.38	Joback Method
dvisc	0.0000291	Pa×s	955.31	Joback Method
dvisc	0.0000380	Pa×s	892.20	Joback Method

dvisc	0.0000518	Pa×s	829.09	Joback Method
dvisc	0.0000743	Pa×s	765.98	Joback Method
dvisc	0.0001137	Pa×s	702.87	Joback Method
dvisc	0.0001892	Pa×s	639.76	Joback Method
dvisc	0.0003520	Pa×s	576.65	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=U369954&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