Diethylmalonic acid, 2-formylphenyl hexyl ester

Inchi: InChI=1S/C20H28O5/c1-4-7-8-11-14-24-18(22)20(5-2,6-3)19(23)25-17-13-10-9-12-16(17

InchiKey: CJUYXHVVLBNZTD-UHFFFAOYSA-N

Formula: C20H28O5

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

Mol. weight [g/mol]: 348.43

Physical Properties

Property code	Value	Unit	Source
gf	-344.22	kJ/mol	Joback Method
hf	-815.00	kJ/mol	Joback Method
hfus	41.66	kJ/mol	Joback Method
hvap	86.79	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.334		Crippen Method
mcvol	285.350	ml/mol	McGowan Method
pc	1438.07	kPa	Joback Method
rinpol	2350.00		NIST Webbook
tb	886.67	K	Joback Method
tc	1096.97	K	Joback Method
tf	542.84	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.39	J/mol×K	886.67	Joback Method
cpg	955.36	J/mol×K	1061.92	Joback Method
cpg	945.28	J/mol×K	1026.87	Joback Method
cpg	934.19	J/mol×K	991.82	Joback Method
cpg	922.04	J/mol×K	956.77	Joback Method
cpg	908.79	J/mol×K	921.72	Joback Method
cpg	964.48	J/mol×K	1096.97	Joback Method
dvisc	0.0000460	Pa×s	886.67	Joback Method
dvisc	0.0000597	Pa×s	829.37	Joback Method

dvisc	0.0000805	Pa×s	772.06	Joback Method
dvisc	0.0001139	Pa×s	714.75	Joback Method
dvisc	0.0001713	Pa×s	657.45	Joback Method
dvisc	0.0002785	Pa×s	600.14	Joback Method
dvisc	0.0005017	Pa×s	542.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369951&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

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