Diethylmalonic acid, decyl 2-formylphenyl ester

Inchi: InChI=1S/C24H36O5/c1-4-7-8-9-10-11-12-15-18-28-22(26)24(5-2,6-3)23(27)29-21-17-14

InchiKey: DVNLBEYAODALJC-UHFFFAOYSA-N

Formula: C24H36O5

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

Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-310.54	kJ/mol	Joback Method
hf	-897.56	kJ/mol	Joback Method
hfus	52.02	kJ/mol	Joback Method
hvap	95.69	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.895		Crippen Method
mcvol	341.710	ml/mol	McGowan Method
pc	1095.72	kPa	Joback Method
rinpol	2745.00		NIST Webbook
tb	978.19	K	Joback Method
tc	1197.99	K	Joback Method
tf	587.92	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.01	J/mol×K	978.19	Joback Method
cpg	1149.23	J/mol×K	1014.82	Joback Method
cpg	1163.14	J/mol×K	1051.46	Joback Method
cpg	1175.79	J/mol×K	1088.09	Joback Method
cpg	1187.26	J/mol×K	1124.72	Joback Method
cpg	1197.60	J/mol×K	1161.36	Joback Method
cpg	1206.89	J/mol×K	1197.99	Joback Method
dvisc	0.0003109	Pa×s	587.92	Joback Method
dvisc	0.0001655	Pa×s	652.97	Joback Method

dvisc	0.0000987	Pa×s	718.01	Joback Method
dvisc	0.0000642	Pa×s	783.06	Joback Method
dvisc	0.0000446	Pa×s	848.10	Joback Method
dvisc	0.0000326	Pa×s	913.14	Joback Method
dvisc	0.0000249	Pa×s	978.19	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=U369955&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