Diethylmalonic acid, decyl 4-methoxyphenyl ester

Inchi: InChI=1S/C24H38O5/c1-5-8-9-10-11-12-13-14-19-28-22(25)24(6-2,7-3)23(26)29-21-17-1

InchiKey: YTXWTWKCZFPUSK-UHFFFAOYSA-N

Formula: C24H38O5

SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(OC)cc1

Mol. weight [g/mol]: 406.56

Physical Properties

Property code	Value	Unit	Source
gf	-316.02	kJ/mol	Joback Method
hf	-944.20	kJ/mol	Joback Method
hfus	50.92	kJ/mol	Joback Method
hvap	91.38	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.091		Crippen Method
mcvol	346.010	ml/mol	McGowan Method
pc	1032.57	kPa	Joback Method
rinpol	2738.00		NIST Webbook
tb	951.95	K	Joback Method
tc	1166.26	K	Joback Method
tf	568.15	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.27	J/mol×K	951.95	Joback Method
cpg	1217.25	J/mol×K	1130.54	Joback Method
cpg	1206.33	J/mol×K	1094.82	Joback Method
cpg	1194.12	J/mol×K	1059.10	Joback Method
cpg	1180.57	J/mol×K	1023.39	Joback Method
cpg	1165.63	J/mol×K	987.67	Joback Method
cpg	1226.92	J/mol×K	1166.26	Joback Method
dvisc	0.0000174	Pa×s	951.95	Joback Method
dvisc	0.0000230	Pa×s	887.98	Joback Method

dvisc	0.0000316	Pa×s	824.02	Joback Method
dvisc	0.0000459	Pa×s	760.05	Joback Method
dvisc	0.0000713	Pa×s	696.08	Joback Method
dvisc	0.0001213	Pa×s	632.12	Joback Method
dvisc	0.0002324	Pa×s	568.15	Joback Method

Sources

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=U369845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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