Diethylmalonic acid, hexyl 3-methoxyphenyl ester

Inchi: InChI=1S/C20H30O5/c1-5-8-9-10-14-24-18(21)20(6-2,7-3)19(22)25-17-13-11-12-16(15-1

InchiKey: IYCOFGBWBMLCBT-UHFFFAOYSA-N

Formula: C20H30O5

SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(OC)c1

Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-349.70	kJ/mol	Joback Method
hf	-861.64	kJ/mol	Joback Method
hfus	40.56	kJ/mol	Joback Method
hvap	82.48	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.530		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	2319.00		NIST Webbook
tb	860.43	K	Joback Method
tc	1066.28	K	Joback Method
tf	523.07	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.95	J/mol×K	860.43	Joback Method
cpg	923.71	J/mol×K	894.74	Joback Method
cpg	938.25	J/mol×K	929.05	Joback Method
cpg	951.60	J/mol×K	963.35	Joback Method
cpg	963.80	J/mol×K	997.66	Joback Method
cpg	974.86	J/mol×K	1031.97	Joback Method
cpg	984.83	J/mol×K	1066.28	Joback Method
dvisc	0.0003761	Pa×s	523.07	Joback Method
dvisc	0.0002048	Pa×s	579.30	Joback Method

dvisc	0.0001242	Pa×s	635.52	Joback Method
dvisc	0.0000817	Pa×s	691.75	Joback Method
dvisc	0.0000572	Pa×s	747.98	Joback Method
dvisc	0.0000421	Pa×s	804.20	Joback Method
dvisc	0.0000323	Pa×s	860.43	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=U370873&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