Diethylmalonic acid, 3-methoxyphenyl nonyl ester

Inchi: InChI=1S/C23H36O5/c1-5-8-9-10-11-12-13-17-27-21(24)23(6-2,7-3)22(25)28-20-16-14-1

InchiKey: ABJUXKSMMRGBAJ-UHFFFAOYSA-N

Formula: C23H36O5

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

Mol. weight [g/mol]: 392.53

Physical Properties

Property code	Value	Unit	Source
gf	-324.44	kJ/mol	Joback Method
hf	-923.56	kJ/mol	Joback Method
hfus	48.33	kJ/mol	Joback Method
hvap	89.16	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.701		Crippen Method
mcvol	331.920	ml/mol	McGowan Method
pc	1099.35	kPa	Joback Method
rinpol	2598.00		NIST Webbook
rinpol	2598.00		NIST Webbook
tb	929.07	K	Joback Method
tc	1139.98	K	Joback Method
tf	556.88	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.08	J/mol×K	929.07	Joback Method
cpg	1155.83	J/mol×K	1104.82	Joback Method
cpg	1144.84	J/mol×K	1069.67	Joback Method
cpg	1132.62	J/mol×K	1034.52	Joback Method
cpg	1119.11	J/mol×K	999.37	Joback Method
cpg	1104.27	J/mol×K	964.22	Joback Method
cpg	1165.60	J/mol×K	1139.98	Joback Method
dvisc	0.0000204	Pa×s	929.07	Joback Method

dvisc	0.0000268	Pa×s	867.04	Joback Method
dvisc	0.0000368	Pa×s	805.01	Joback Method
dvisc	0.0000532	Pa×s	742.98	Joback Method
dvisc	0.0000822	Pa×s	680.94	Joback Method
dvisc	0.0001388	Pa×s	618.91	Joback Method
dvisc	0.0002633	Pa×s	556.88	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=U370876&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