Diethylmalonic acid, heptyl 3-methoxyphenyl ester

Inchi: InChI=1S/C21H32O5/c1-5-8-9-10-11-15-25-19(22)21(6-2,7-3)20(23)26-18-14-12-13-17(1

InchiKey: KPZVOJBSILZJMW-UHFFFAOYSA-N

Formula: C21H32O5

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

Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-341.28	kJ/mol	Joback Method
hf	-882.28	kJ/mol	Joback Method
hfus	43.15	kJ/mol	Joback Method
hvap	84.70	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.921		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
rinpol	2412.00		NIST Webbook
tb	883.31	K	Joback Method
tc	1090.05	K	Joback Method
tf	534.34	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.36	J/mol×K	883.31	Joback Method
cpg	1034.59	J/mol×K	1055.59	Joback Method
cpg	1023.53	J/mol×K	1021.13	Joback Method
cpg	1011.31	J/mol×K	986.68	Joback Method
cpg	997.90	J/mol×K	952.22	Joback Method
cpg	983.26	J/mol×K	917.77	Joback Method
cpg	1044.52	J/mol×K	1090.05	Joback Method
dvisc	0.0000277	Pa×s	883.31	Joback Method
dvisc	0.0000363	Pa×s	825.15	Joback Method

dvisc	0.0000495	Pa×s	766.99	Joback Method
dvisc	0.0000710	Pa×s	708.82	Joback Method
dvisc	0.0001085	Pa×s	650.66	Joback Method
dvisc	0.0001804	Pa×s	592.50	Joback Method
dvisc	0.0003350	Pa×s	534.34	Joback Method

Sources

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=U370874&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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