Diethylmalonic acid, butyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C20H30O5/c1-6-9-14-23-18(21)20(7-2,8-3)19(22)25-17-13-11-10-12-16(17)24-

InchiKey: GAUYBNIAYCWWOG-UHFFFAOYSA-N

Formula: C20H30O5

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-352.14	kJ/mol	Joback Method
hf	-866.92	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	82.09	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.529		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
tb	859.99	K	Joback Method
tc	1067.72	K	Joback Method
tf	508.07	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.47	J/mol×K	859.99	Joback Method
cpg	924.35	J/mol×K	894.61	Joback Method
cpg	938.98	J/mol×K	929.23	Joback Method
cpg	952.39	J/mol×K	963.86	Joback Method
cpg	964.61	J/mol×K	998.48	Joback Method
cpg	975.68	J/mol×K	1033.10	Joback Method
cpg	985.60	J/mol×K	1067.72	Joback Method
dvisc	0.0004263	Pa×s	508.07	Joback Method

dvisc	0.0002171	Pa×s	566.72	Joback Method
dvisc	0.0001255	Pa×s	625.38	Joback Method
dvisc	0.0000797	Pa×s	684.03	Joback Method
dvisc	0.0000543	Pa×s	742.68	Joback Method
dvisc	0.0000392	Pa×s	801.34	Joback Method
dvisc	0.0000296	Pa×s	859.99	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=U369584&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