Diethylmalonic acid, 2-isopropoxyphenyl octyl ester

Inchi: InChI=1S/C24H38O5/c1-6-9-10-11-12-15-18-27-22(25)24(7-2,8-3)23(26)29-21-17-14-13-

InchiKey: XYDRVFWOAQUAHT-UHFFFAOYSA-N

Formula: C24H38O5

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

Mol. weight [g/mol]: 406.56

Physical Properties

Property code	Value	Unit	Source
gf	-318.46	kJ/mol	Joback Method
hf	-949.48	kJ/mol	Joback Method
hfus	47.39	kJ/mol	Joback Method
hvap	90.99	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.089		Crippen Method
mcvol	346.010	ml/mol	McGowan Method
pc	1037.90	kPa	Joback Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
tb	951.51	K	Joback Method
tc	1166.29	K	Joback Method
tf	553.15	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.68	J/mol×K	951.51	Joback Method
cpg	1217.44	J/mol×K	1130.49	Joback Method
cpg	1206.60	J/mol×K	1094.69	Joback Method
cpg	1194.45	J/mol×K	1058.90	Joback Method
cpg	1180.95	J/mol×K	1023.10	Joback Method
cpg	1166.04	J/mol×K	987.31	Joback Method
cpg	1227.00	J/mol×K	1166.29	Joback Method
dvisc	0.0000159	Pa×s	951.51	Joback Method

dvisc	0.0000212	Pa×s	885.12	Joback Method
dvisc	0.0000298	Pa×s	818.72	Joback Method
dvisc	0.0000443	Pa×s	752.33	Joback Method
dvisc	0.0000712	Pa×s	685.94	Joback Method
dvisc	0.0001268	Pa×s	619.54	Joback Method
dvisc	0.0002591	Pa×s	553.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369588&Units=SI
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

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