Diethylmalonic acid, 2-isopropylphenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C23H36O4/c1-8-13-19(17(6)7)26-21(24)23(9-2,10-3)22(25)27-20-15-12-11-14-

InchiKey: IISMGNKGGVHUQB-UHFFFAOYSA-N

Formula: C23H36O4

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)Oc1ccccc1C(C)C)C(C)C

Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-226.76	kJ/mol	Joback Method
hf	-807.18	kJ/mol	Joback Method
hfus	36.57	kJ/mol	Joback Method
hvap	85.58	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.890		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
tb	905.33	K	Joback Method
tc	1117.42	K	Joback Method
tf	489.65	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.80	J/mol×K	905.33	Joback Method
cpg	1132.24	J/mol×K	1082.07	Joback Method
cpg	1120.19	J/mol×K	1046.72	Joback Method
cpg	1106.98	J/mol×K	1011.38	Joback Method
cpg	1092.55	J/mol×K	976.03	Joback Method
cpg	1076.84	J/mol×K	940.68	Joback Method
cpg	1143.17	J/mol×K	1117.42	Joback Method
dvisc	0.0000211	Pa×s	905.33	Joback Method

dvisc	0.0000291	Pa×s	836.05	Joback Method
dvisc	0.0000428	Pa×s	766.77	Joback Method
dvisc	0.0000677	Pa×s	697.49	Joback Method
dvisc	0.0001187	Pa×s	628.21	Joback Method
dvisc	0.0002391	Pa×s	558.93	Joback Method
dvisc	0.0005871	Pa×s	489.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369970&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