Diethylmalonic acid, 2-isopropoxyphenyl tridecyl ester

Inchi: InChI=1S/C29H48O5/c1-6-9-10-11-12-13-14-15-16-17-20-23-32-27(30)29(7-2,8-3)28(31)
InchiKey: WSCJOSDFYYVLSZ-UHFFFAOYSA-N
Formula: C29H48O5
SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 476.69

Physical Properties

Property code	Value	Unit	Source
gf	-276.36	kJ/mol	Joback Method
hf	-1052.68	kJ/mol	Joback Method
hfus	60.34	kJ/mol	Joback Method
hvap	102.12	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	8.040		Crippen Method
mcvol	416.460	ml/mol	McGowan Method
pc	778.51	kPa	Joback Method
rinpol	3049.00		NIST Webbook
rinpol	3049.00		NIST Webbook
tb	1065.91	K	Joback Method
tc	1311.45	K	Joback Method
tf	609.50	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1461.72	J/mol×K	1065.91	Joback Method
cpg	1479.08	J/mol×K	1106.83	Joback Method
cpg	1494.49	J/mol×K	1147.76	Joback Method
cpg	1508.05	J/mol×K	1188.68	Joback Method
cpg	1519.85	J/mol×K	1229.60	Joback Method
cpg	1529.98	J/mol×K	1270.52	Joback Method
cpg	1538.53	J/mol×K	1311.45	Joback Method
dvisc	0.0001312	Pa×s	609.50	Joback Method

dvisc	0.0000615	Pa×s	685.57	Joback Method
dvisc	0.0000336	Pa×s	761.64	Joback Method
dvisc	0.0000204	Pa×s	837.70	Joback Method
dvisc	0.0000135	Pa×s	913.77	Joback Method
dvisc	0.0000095	Pa×s	989.84	Joback Method
dvisc	0.0000071	Pa×s	1065.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369591&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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