

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:	CCCCCCCCCCCCOC(=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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000615	Paxs	685.57	Joback Method
dvisc	0.0000336	Paxs	761.64	Joback Method
dvisc	0.0000204	Paxs	837.70	Joback Method
dvisc	0.0000135	Paxs	913.77	Joback Method
dvisc	0.0000095	Paxs	989.84	Joback Method
dvisc	0.0000071	Paxs	1065.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U369591&Units=SI

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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