

Diethylmalonic acid, dodecyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C28H46O5/c1-6-9-10-11-12-13-14-15-16-19-22-31-26(29)28(7-2,8-3)27(30)33
InchiKey: AILOXQJJLDPFGT-UHFFFAOYSA-N
Formula: C28H46O5
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 462.66

Physical Properties

Property code	Value	Unit	Source
gf	-284.78	kJ/mol	Joback Method
hf	-1032.04	kJ/mol	Joback Method
hfus	57.75	kJ/mol	Joback Method
hvap	99.90	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.650		Crippen Method
mcvol	402.370	ml/mol	McGowan Method
pc	821.95	kPa	Joback Method
rinsol	2944.00		NIST Webbook
tb	1043.03	K	Joback Method
tc	1280.08	K	Joback Method
tf	598.23	K	Joback Method
vc	1.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1398.64	J/molxK	1043.03	Joback Method
cpg	1415.74	J/molxK	1082.54	Joback Method
cpg	1431.02	J/molxK	1122.05	Joback Method
cpg	1444.57	J/molxK	1161.55	Joback Method
cpg	1456.47	J/molxK	1201.06	Joback Method
cpg	1466.78	J/molxK	1240.57	Joback Method
cpg	1475.59	J/molxK	1280.08	Joback Method
dvisc	0.0001510	Paxs	598.23	Joback Method
dvisc	0.0000714	Paxs	672.36	Joback Method

dvisc	0.0000392	Paxs	746.50	Joback Method
dvisc	0.0000239	Paxs	820.63	Joback Method
dvisc	0.0000159	Paxs	894.76	Joback Method
dvisc	0.0000112	Paxs	968.90	Joback Method
dvisc	0.0000083	Paxs	1043.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U369590&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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