

Dimethylmalonic acid, isohexyl 3-phenylpropyl ester

Inchi:	InChI=1S/C20H30O4/c1-16(2)10-8-14-23-18(21)20(3,4)19(22)24-15-9-13-17-11-6-5-7-12
InchiKey:	FYKFEWPHNGZLLS-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CC(C)CCCOC(=O)C(C)(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-237.51	kJ/mol	Joback Method
hf	-723.23	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.168		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinsol	2189.00		NIST Webbook
tb	832.59	K	Joback Method
tc	1039.11	K	Joback Method
tf	473.32	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.92	J/molxK	832.59	Joback Method
cpg	951.25	J/molxK	1004.69	Joback Method
cpg	939.17	J/molxK	970.27	Joback Method
cpg	926.04	J/molxK	935.85	Joback Method
cpg	911.82	J/molxK	901.43	Joback Method
cpg	896.46	J/molxK	867.01	Joback Method
cpg	962.34	J/molxK	1039.11	Joback Method
dvisc	0.0000394	Paxs	832.59	Joback Method
dvisc	0.0000533	Paxs	772.71	Joback Method

dvisc	0.0000758	Paxs	712.83	Joback Method
dvisc	0.0001150	Paxs	652.95	Joback Method
dvisc	0.0001899	Paxs	593.08	Joback Method
dvisc	0.0003508	Paxs	533.20	Joback Method
dvisc	0.0007571	Paxs	473.32	Joback Method

Sources

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=U361834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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