

Dimethylmalonic acid, hexyl 3-phenylpropyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-235.07	kJ/mol	Joback Method
hf	-717.95	kJ/mol	Joback Method
hfus	39.76	kJ/mol	Joback Method
hvap	79.41	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.312		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	2228.00		NIST Webbook
tb	833.03	K	Joback Method
tc	1037.37	K	Joback Method
tf	488.32	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.40	J/molxK	833.03	Joback Method
cpg	895.78	J/molxK	867.09	Joback Method
cpg	911.01	J/molxK	901.14	Joback Method
cpg	925.14	J/molxK	935.20	Joback Method
cpg	938.20	J/molxK	969.25	Joback Method
cpg	950.26	J/molxK	1003.31	Joback Method
cpg	961.35	J/molxK	1037.37	Joback Method
dvisc	0.0006491	Paxs	488.32	Joback Method
dvisc	0.0003253	Paxs	545.77	Joback Method

dvisc	0.0001860	Paxs	603.22	Joback Method
dvisc	0.0001172	Paxs	660.67	Joback Method
dvisc	0.0000795	Paxs	718.13	Joback Method
dvisc	0.0000571	Paxs	775.58	Joback Method
dvisc	0.0000430	Paxs	833.03	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=U361835&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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