

Dimethylmalonic acid, isobutyl 2-phenethyl ester

Inchi:	InChI=1S/C17H24O4/c1-13(2)12-21-16(19)17(3,4)15(18)20-11-10-14-8-6-5-7-9-14/h5-9,
InchiKey:	HMQJKTZMOGBQEN-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CC(C)COC(=O)C(C)(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-262.77	kJ/mol	Joback Method
hf	-661.31	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	72.34	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.998		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	1883.00		NIST Webbook
tb	763.95	K	Joback Method
tc	974.55	K	Joback Method
tf	439.51	K	Joback Method
vc	0.910	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.52	J/molxK	763.95	Joback Method
cpg	723.59	J/molxK	799.05	Joback Method
cpg	738.52	J/molxK	834.15	Joback Method
cpg	752.35	J/molxK	869.25	Joback Method
cpg	765.13	J/molxK	904.35	Joback Method
cpg	776.88	J/molxK	939.45	Joback Method
cpg	787.66	J/molxK	974.55	Joback Method
dvisc	0.0010708	Paxs	439.51	Joback Method
dvisc	0.0005121	Paxs	493.58	Joback Method

dvisc	0.0002833	Paxs	547.66	Joback Method
dvisc	0.0001743	Paxs	601.73	Joback Method
dvisc	0.0001162	Paxs	655.80	Joback Method
dvisc	0.0000824	Paxs	709.88	Joback Method
dvisc	0.0000613	Paxs	763.95	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=U361615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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