

Dimethylmalonic acid, ethyl 4-(4-methoxyphenyl)cyclohexyl ester

Inchi:	InChI=1S/C20H28O5/c1-5-24-18(21)20(2,3)19(22)25-17-12-8-15(9-13-17)14-6-10-16(23)
InchiKey:	QHDM LQSUPJZCDF-UHFFFAOYSA-N
Formula:	C20H28O5
SMILES:	CCOC(=O)C(C)(C)C(=O)OC1CCC(c2ccc(OC)cc2)CC1
Mol. weight [g/mol]:	348.43

Physical Properties

Property code	Value	Unit	Source
gf	-332.96	kJ/mol	Joback Method
hf	-827.66	kJ/mol	Joback Method
hfus	33.46	kJ/mol	Joback Method
hvap	82.60	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.854		Crippen Method
mcvol	278.790	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinsol	2621.00		NIST Webbook
tb	875.31	K	Joback Method
tc	1101.28	K	Joback Method
tf	526.21	K	Joback Method
vc	1.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.86	J/molxK	875.31	Joback Method
cpg	923.71	J/molxK	912.97	Joback Method
cpg	938.89	J/molxK	950.63	Joback Method
cpg	952.44	J/molxK	988.29	Joback Method
cpg	964.39	J/molxK	1025.95	Joback Method
cpg	974.77	J/molxK	1063.62	Joback Method
cpg	983.61	J/molxK	1101.28	Joback Method
dvisc	0.0004716	Paxs	526.21	Joback Method
dvisc	0.0002598	Paxs	584.39	Joback Method

dvisc	0.0001594	Paxs	642.58	Joback Method
dvisc	0.0001061	Paxs	700.76	Joback Method
dvisc	0.0000752	Paxs	758.94	Joback Method
dvisc	0.0000559	Paxs	817.13	Joback Method
dvisc	0.0000433	Paxs	875.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363914&Units=SI
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

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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