

Dimethylmalonic acid, ethyl 1-phenyl-2-(cyclohex-2-enyl)ethyl ester

Inchi:	InChI=1S/C21H28O4/c1-4-24-19(22)21(2,3)20(23)25-18(17-13-9-6-10-14-17)15-16-11-7
InchiKey:	ZBUBJFIHRVBRSG-UHFFFAOYSA-N
Formula:	C21H28O4
SMILES:	CCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]:	344.44

Physical Properties

Property code	Value	Unit	Source
gf	-174.68	kJ/mol	Joback Method
hf	-631.77	kJ/mol	Joback Method
hfus	31.88	kJ/mol	Joback Method
hvap	81.97	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.607		Crippen Method
mcvol	282.710	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	2230.00		NIST Webbook
tb	874.18	K	Joback Method
tc	1103.02	K	Joback Method
tf	492.73	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.26	J/molxK	874.18	Joback Method
cpg	922.07	J/molxK	912.32	Joback Method
cpg	937.35	J/molxK	950.46	Joback Method
cpg	951.17	J/molxK	988.60	Joback Method
cpg	963.61	J/molxK	1026.74	Joback Method
cpg	974.74	J/molxK	1064.88	Joback Method
cpg	984.62	J/molxK	1103.02	Joback Method
dvisc	0.0007396	Paxs	492.73	Joback Method
dvisc	0.0003389	Paxs	556.31	Joback Method

dvisc	0.0001822	Paxs	619.88	Joback Method
dvisc	0.0001100	Paxs	683.45	Joback Method
dvisc	0.0000723	Paxs	747.03	Joback Method
dvisc	0.0000508	Paxs	810.61	Joback Method
dvisc	0.0000376	Paxs	874.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361868&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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