

Diethylmalonic acid, diphenethyl ester

Inchi:	InChI=1S/C23H28O4/c1-3-23(4-2,21(24)26-17-15-19-11-7-5-8-12-19)22(25)27-18-16-20
InchiKey:	YWCMSYJIHQOLSO-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CCC(CC)(C(=O)OCCc1ccccc1)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-97.40	kJ/mol	Joback Method
hf	-543.34	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	88.36	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.365		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2571.00		NIST Webbook
tb	928.35	K	Joback Method
tc	1154.94	K	Joback Method
tf	548.55	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.49	J/molxK	928.35	Joback Method
cpg	973.24	J/molxK	966.11	Joback Method
cpg	986.70	J/molxK	1003.88	Joback Method
cpg	998.94	J/molxK	1041.64	Joback Method
cpg	1010.05	J/molxK	1079.41	Joback Method
cpg	1020.11	J/molxK	1117.17	Joback Method
cpg	1029.21	J/molxK	1154.94	Joback Method
dvisc	0.0003826	Paxs	548.55	Joback Method
dvisc	0.0001970	Paxs	611.85	Joback Method

dvisc	0.0001148	Paxs	675.15	Joback Method
dvisc	0.0000735	Paxs	738.45	Joback Method
dvisc	0.0000504	Paxs	801.75	Joback Method
dvisc	0.0000366	Paxs	865.05	Joback Method
dvisc	0.0000277	Paxs	928.35	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=U369561&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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