

Diethylmalonic acid, ethyl phenethyl ester

Inchi:	InChI=1S/C17H24O4/c1-4-17(5-2,15(18)20-6-3)16(19)21-13-12-14-10-8-7-9-11-14/h7-11
InchiKey:	JZUMBTVPMDETQG-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-260.33	kJ/mol	Joback Method
hf	-656.03	kJ/mol	Joback Method
hfus	31.99	kJ/mol	Joback Method
hvap	72.73	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.142		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	1889.00		NIST Webbook
tb	764.39	K	Joback Method
tc	971.89	K	Joback Method
tf	454.51	K	Joback Method
vc	0.916	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.97	J/molxK	764.39	Joback Method
cpg	722.81	J/molxK	798.97	Joback Method
cpg	737.54	J/molxK	833.56	Joback Method
cpg	751.22	J/molxK	868.14	Joback Method
cpg	763.87	J/molxK	902.73	Joback Method
cpg	775.55	J/molxK	937.31	Joback Method
cpg	786.29	J/molxK	971.89	Joback Method
dvisc	0.0009021	Paxs	454.51	Joback Method
dvisc	0.0004682	Paxs	506.16	Joback Method

dvisc	0.0002743	Paxs	557.80	Joback Method
dvisc	0.0001760	Paxs	609.45	Joback Method
dvisc	0.0001210	Paxs	661.10	Joback Method
dvisc	0.0000879	Paxs	712.74	Joback Method
dvisc	0.0000666	Paxs	764.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369545&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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