

Diethylmalonic acid, 1-phenylpropyl propyl ester

Inchi:	InChI=1S/C19H28O4/c1-5-14-22-17(20)19(7-3,8-4)18(21)23-16(6-2)15-12-10-9-11-13-15
InchiKey:	LZCDIRBKEVVVJB-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-245.93	kJ/mol	Joback Method
hf	-702.59	kJ/mol	Joback Method
hfus	33.64	kJ/mol	Joback Method
hvap	76.79	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.441		Crippen Method
mvol	269.690	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	1955.00		NIST Webbook
tb	809.71	K	Joback Method
tc	1016.99	K	Joback Method
tf	462.05	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.57	J/molxK	809.71	Joback Method
cpg	837.98	J/molxK	844.26	Joback Method
cpg	853.22	J/molxK	878.80	Joback Method
cpg	867.33	J/molxK	913.35	Joback Method
cpg	880.36	J/molxK	947.89	Joback Method
cpg	892.36	J/molxK	982.44	Joback Method
cpg	903.37	J/molxK	1016.99	Joback Method
dvisc	0.0008531	Paxs	462.05	Joback Method
dvisc	0.0003993	Paxs	519.99	Joback Method

dvisc	0.0002176	Paxs	577.94	Joback Method
dvisc	0.0001325	Paxs	635.88	Joback Method
dvisc	0.0000876	Paxs	693.82	Joback Method
dvisc	0.0000618	Paxs	751.77	Joback Method
dvisc	0.0000458	Paxs	809.71	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=U370189&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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