

Diethylmalonic acid, 3-phenylpropyl propyl ester

Inchi:	InChI=1S/C19H28O4/c1-4-14-22-17(20)19(5-2,6-3)18(21)23-15-10-13-16-11-8-7-9-12-16
InchiKey:	XLKCAQRRXUZDIB-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-243.49	kJ/mol	Joback Method
hf	-697.31	kJ/mol	Joback Method
hfus	37.17	kJ/mol	Joback Method
hvap	77.18	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.922		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	2126.00		NIST Webbook
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tb	810.15	K	Joback Method
tc	1014.93	K	Joback Method
tf	477.05	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.04	J/molxK	810.15	Joback Method
cpg	891.24	J/molxK	980.80	Joback Method
cpg	879.29	J/molxK	946.67	Joback Method
cpg	866.33	J/molxK	912.54	Joback Method
cpg	852.34	J/molxK	878.41	Joback Method
cpg	837.26	J/molxK	844.28	Joback Method
cpg	902.23	J/molxK	1014.93	Joback Method
dvisc	0.0000498	Paxs	810.15	Joback Method

dvisc	0.0000661	Paxs	754.63	Joback Method
dvisc	0.0000917	Paxs	699.12	Joback Method
dvisc	0.0001346	Paxs	643.60	Joback Method
dvisc	0.0002124	Paxs	588.08	Joback Method
dvisc	0.0003686	Paxs	532.57	Joback Method
dvisc	0.0007273	Paxs	477.05	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=U369651&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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