

Diethylmalonic acid, 4-biphenyl octyl ester

Inchi:	InChI=1S/C27H36O4/c1-4-7-8-9-10-14-21-30-25(28)27(5-2,6-3)26(29)31-24-19-17-23(18)
InchiKey:	ZKKRXORKZIIHHGX-UHFFFAOYSA-N
Formula:	C27H36O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	424.57

Physical Properties

Property code	Value	Unit	Source
gf	-73.35	kJ/mol	Joback Method
hf	-637.37	kJ/mol	Joback Method
hfus	51.54	kJ/mol	Joback Method
hvap	97.93	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	6.969		Crippen Method
mvol	358.650	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	3115.00		NIST Webbook
tb	1024.85	K	Joback Method
tc	1256.82	K	Joback Method
tf	606.15	K	Joback Method
vc	1.369	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.09	J/molxK	1024.85	Joback Method
cpg	1261.23	J/molxK	1218.16	Joback Method
cpg	1251.15	J/molxK	1179.50	Joback Method
cpg	1239.99	J/molxK	1140.84	Joback Method
cpg	1227.66	J/molxK	1102.17	Joback Method
cpg	1214.06	J/molxK	1063.51	Joback Method
cpg	1270.33	J/molxK	1256.82	Joback Method
dvisc	0.0000152	Paxs	1024.85	Joback Method
dvisc	0.0000200	Paxs	955.07	Joback Method

dvisc	0.0000275	Paxs	885.28	Joback Method
dvisc	0.0000398	Paxs	815.50	Joback Method
dvisc	0.0000619	Paxs	745.72	Joback Method
dvisc	0.0001055	Paxs	675.93	Joback Method
dvisc	0.0002031	Paxs	606.15	Joback Method

Sources

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=U370428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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