

Diethylmalonic acid, 4-biphenyl nonyl ester

Inchi:	InChI=1S/C28H38O4/c1-4-7-8-9-10-11-15-22-31-26(29)28(5-2,6-3)27(30)32-25-20-18-24
InchiKey:	KWGOMGGWKJNEOR-UHFFFAOYSA-N
Formula:	C28H38O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	438.60

Physical Properties

Property code	Value	Unit	Source
gf	-64.93	kJ/mol	Joback Method
hf	-658.01	kJ/mol	Joback Method
hfus	54.13	kJ/mol	Joback Method
hvap	100.15	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	7.359		Crippen Method
mcvol	372.740	ml/mol	McGowan Method
pc	1009.09	kPa	Joback Method
rinpol	3210.00		NIST Webbook
tb	1047.73	K	Joback Method
tc	1283.24	K	Joback Method
tf	617.42	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1260.72	J/molxK	1047.73	Joback Method
cpg	1275.84	J/molxK	1086.98	Joback Method
cpg	1289.56	J/molxK	1126.23	Joback Method
cpg	1301.99	J/molxK	1165.48	Joback Method
cpg	1313.24	J/molxK	1204.73	Joback Method
cpg	1323.40	J/molxK	1243.98	Joback Method
cpg	1332.59	J/molxK	1283.24	Joback Method
dvisc	0.0001784	Paxs	617.42	Joback Method
dvisc	0.0000918	Paxs	689.14	Joback Method

dvisc	0.0000536	Paxs	760.86	Joback Method
dvisc	0.0000343	Paxs	832.58	Joback Method
dvisc	0.0000236	Paxs	904.29	Joback Method
dvisc	0.0000171	Paxs	976.01	Joback Method
dvisc	0.0000130	Paxs	1047.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370429&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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