

Diethylmalonic acid, 4-biphenyl pentyl ester

Inchi:	InChI=1S/C24H30O4/c1-4-7-11-18-27-22(25)24(5-2,6-3)23(26)28-21-16-14-20(15-17-21
InchiKey:	LQNPOXNNVNMFJC-UHFFFAOYSA-N
Formula:	C24H30O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	382.49

Physical Properties

Property code	Value	Unit	Source
gf	-98.61	kJ/mol	Joback Method
hf	-575.45	kJ/mol	Joback Method
hfus	43.77	kJ/mol	Joback Method
hvap	91.25	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	5.799		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1308.95	kPa	Joback Method
rinsol	2818.00		NIST Webbook
tb	956.21	K	Joback Method
tc	1183.42	K	Joback Method
tf	572.34	K	Joback Method
vc	1.200	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.05	J/molxK	956.21	Joback Method
cpg	1078.16	J/molxK	1145.55	Joback Method
cpg	1068.25	J/molxK	1107.68	Joback Method
cpg	1057.27	J/molxK	1069.81	Joback Method
cpg	1045.13	J/molxK	1031.95	Joback Method
cpg	1031.75	J/molxK	994.08	Joback Method
cpg	1087.06	J/molxK	1183.42	Joback Method
dvisc	0.0000242	Paxs	956.21	Joback Method
dvisc	0.0000317	Paxs	892.23	Joback Method

dvisc	0.0000431	Paxs	828.25	Joback Method
dvisc	0.0000618	Paxs	764.28	Joback Method
dvisc	0.0000946	Paxs	700.30	Joback Method
dvisc	0.0001578	Paxs	636.32	Joback Method
dvisc	0.0002952	Paxs	572.34	Joback Method

Sources

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=U370424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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