

Diethylmalonic acid, 4-biphenyl hexyl ester

Inchi:	InChI=1S/C25H32O4/c1-4-7-8-12-19-28-23(26)25(5-2,6-3)24(27)29-22-17-15-21(16-18-2
InchiKey:	PHVWOEKYNXPPMB-UHFFFAOYSA-N
Formula:	C25H32O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	396.52

Physical Properties

Property code	Value	Unit	Source
gf	-90.19	kJ/mol	Joback Method
hf	-596.09	kJ/mol	Joback Method
hfus	46.36	kJ/mol	Joback Method
hvap	93.47	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	6.189		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1222.55	kPa	Joback Method
rinsol	2920.00		NIST Webbook
tb	979.09	K	Joback Method
tc	1206.97	K	Joback Method
tf	583.61	K	Joback Method
vc	1.256	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1077.22	J/molxK	979.09	Joback Method
cpg	1091.98	J/molxK	1017.07	Joback Method
cpg	1105.42	J/molxK	1055.05	Joback Method
cpg	1117.61	J/molxK	1093.03	Joback Method
cpg	1128.64	J/molxK	1131.01	Joback Method
cpg	1138.60	J/molxK	1168.99	Joback Method
cpg	1147.56	J/molxK	1206.97	Joback Method
dvisc	0.0002613	Paxs	583.61	Joback Method
dvisc	0.0001383	Paxs	649.52	Joback Method

dvisc	0.0000824	Paxs	715.44	Joback Method
dvisc	0.0000535	Paxs	781.35	Joback Method
dvisc	0.0000372	Paxs	847.26	Joback Method
dvisc	0.0000272	Paxs	913.18	Joback Method
dvisc	0.0000208	Paxs	979.09	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=U370426&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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