

Diethylmalonic acid, 4-biphenyl isobutyl ester

Inchi:	InChI=1S/C23H28O4/c1-5-23(6-2,21(24)26-16-17(3)4)22(25)27-20-14-12-19(13-15-20)1
InchiKey:	QOLDFIOUOAPFKA-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-109.47	kJ/mol	Joback Method
hf	-560.09	kJ/mol	Joback Method
hfus	37.66	kJ/mol	Joback Method
hvap	88.63	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.265		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinsol	2644.00		NIST Webbook
tb	932.89	K	Joback Method
tc	1162.62	K	Joback Method
tf	546.07	K	Joback Method
vc	1.139	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.92	J/molxK	932.89	Joback Method
cpg	972.67	J/molxK	971.18	Joback Method
cpg	986.06	J/molxK	1009.47	Joback Method
cpg	998.18	J/molxK	1047.75	Joback Method
cpg	1009.10	J/molxK	1086.04	Joback Method
cpg	1018.91	J/molxK	1124.33	Joback Method
cpg	1027.67	J/molxK	1162.62	Joback Method
dvisc	0.0003692	Paxs	546.07	Joback Method
dvisc	0.0001874	Paxs	610.54	Joback Method

dvisc	0.0001083	Paxs	675.01	Joback Method
dvisc	0.0000688	Paxs	739.48	Joback Method
dvisc	0.0000471	Paxs	803.95	Joback Method
dvisc	0.0000340	Paxs	868.42	Joback Method
dvisc	0.0000258	Paxs	932.89	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=U370390&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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