Diethylmalonic acid, 4-biphenyl butyl ester

Inchi: InChI=1S/C23H28O4/c1-4-7-17-26-21(24)23(5-2,6-3)22(25)27-20-15-13-19(14-16-20)18-
InchiKey: VUBDJSFJJOBDMT-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-107.03	kJ/mol	Joback Method
hf	-554.81	kJ/mol	Joback Method
hfus	41.18	kJ/mol	Joback Method
hvap	89.02	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.409		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinpol	2689.00		NIST Webbook
rinpol	2689.00		NIST Webbook
tb	933.33	K	Joback Method
tc	1160.71	K	Joback Method
tf	561.07	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.45	J/mol×K	933.33	Joback Method
cpg	972.10	J/mol×K	971.23	Joback Method
cpg	985.43	J/mol×K	1009.12	Joback Method
cpg	997.53	J/mol×K	1047.02	Joback Method
cpg	1008.46	J/mol×K	1084.91	Joback Method
cpg	1018.32	J/mol×K	1122.81	Joback Method
cpg	1027.16	J/mol×K	1160.71	Joback Method
dvisc	0.0003324	Pa×s	561.07	Joback Method

dvisc	0.0001796	Pa×s	623.11	Joback Method
dvisc	0.0001085	Pa×s	685.16	Joback Method
dvisc	0.0000713	Pa×s	747.20	Joback Method
dvisc	0.0000499	Pa×s	809.24	Joback Method
dvisc	0.0000368	Pa×s	871.29	Joback Method
dvisc	0.0000282	Pa×s	933.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370391&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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