Diethylmalonic acid, di(1-phenylpropyl) ester

Inchi: InChI=1S/C25H32O4/c1-5-21(19-15-11-9-12-16-19)28-23(26)25(7-3,8-4)24(27)29-22(6-2
InchiKey: PSQVCHZPWRKXTJ-UHFFFAOYSA-N
Formula: C25H32O4
SMILES: CCC(OC(=O)C(CC)(CC)C(=O)OC(CC)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-85.44	kJ/mol	Joback Method
hf	-595.18	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	92.04	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.182		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1249.49	kPa	Joback Method
rinpol	2497.00		NIST Webbook
tb	973.23	K	Joback Method
tc	1203.66	K	Joback Method
tf	541.09	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.03	J/mol×K	973.23	Joback Method
cpg	1141.20	J/mol×K	1165.25	Joback Method
cpg	1131.14	J/mol×K	1126.85	Joback Method
cpg	1119.98	J/mol×K	1088.44	Joback Method
cpg	1107.64	J/mol×K	1050.04	Joback Method
cpg	1094.03	J/mol×K	1011.63	Joback Method
cpg	1150.28	J/mol×K	1203.66	Joback Method
dvisc	0.0000169	Pa×s	973.23	Joback Method
dvisc	0.0000230	Pa×s	901.21	Joback Method

dvisc	0.0000331	Pa×s	829.18	Joback Method
dvisc	0.0000512	Pa×s	757.16	Joback Method
dvisc	0.0000865	Pa×s	685.14	Joback Method
dvisc	0.0001655	Pa×s	613.11	Joback Method
dvisc	0.0003764	Pa×s	541.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370192&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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