Diethylmalonic acid, di(3-phenylpropyl) ester

Inchi: InChI=1S/C25H32O4/c1-3-25(4-2,23(26)28-19-11-17-21-13-7-5-8-14-21)24(27)29-20-12-
InchiKey: LZULVRCRCYLJAK-UHFFFAOYSA-N
Formula: C25H32O4
SMILES: CCC(CC)(C(=O)OCCCc1ccccc1)C(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-80.56	kJ/mol	Joback Method
hf	-584.62	kJ/mol	Joback Method
hfus	46.75	kJ/mol	Joback Method
hvap	92.81	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.145		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1235.48	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	974.11	K	Joback Method
tc	1201.12	K	Joback Method
tf	571.09	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.22	J/mol×K	974.11	Joback Method
cpg	1093.11	J/mol×K	1011.95	Joback Method
cpg	1106.70	J/mol×K	1049.78	Joback Method
cpg	1119.07	J/mol×K	1087.62	Joback Method
cpg	1130.32	J/mol×K	1125.45	Joback Method
cpg	1140.54	J/mol×K	1163.29	Joback Method
cpg	1149.82	J/mol×K	1201.12	Joback Method
dvisc	0.0002985	Pa×s	571.09	Joback Method

dvisc	0.0001507	Pa×s	638.26	Joback Method
dvisc	0.0000867	Pa×s	705.43	Joback Method
dvisc	0.0000549	Pa×s	772.60	Joback Method
dvisc	0.0000374	Pa×s	839.77	Joback Method
dvisc	0.0000270	Pa×s	906.94	Joback Method
dvisc	0.0000203	Pa×s	974.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369668&Units=SI

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