Diethylmalonic acid, 2-methylhex-3-yl 3-phenylpropyl ester

Inchi: InChI=1S/C23H36O4/c1-6-13-20(18(4)5)27-22(25)23(7-2,8-3)21(24)26-17-12-16-19-14-1

InchiKey: JCJIRWUYRDZZRU-UHFFFAOYSA-N

Formula: C23H36O4

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)OCCCc1ccccc1)C(C)C

Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-214.69	kJ/mol	Joback Method
hf	-790.43	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	85.31	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.337		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2375.00		NIST Webbook
tb	900.79	K	Joback Method
tc	1110.53	K	Joback Method
tf	492.13	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.90	J/mol×K	900.79	Joback Method
cpg	1076.96	J/mol×K	935.75	Joback Method
cpg	1092.72	J/mol×K	970.70	Joback Method
cpg	1107.25	J/mol×K	1005.66	Joback Method
cpg	1120.61	J/mol×K	1040.62	Joback Method
cpg	1132.85	J/mol×K	1075.57	Joback Method
cpg	1144.04	J/mol×K	1110.53	Joback Method
dvisc	0.0006055	Pa×s	492.13	Joback Method
dvisc	0.0002511	Pa×s	560.24	Joback Method

dvisc	0.0001261	Pa×s	628.35	Joback Method
dvisc	0.0000724	Pa×s	696.46	Joback Method
dvisc	0.0000459	Pa×s	764.57	Joback Method
dvisc	0.0000314	Pa×s	832.68	Joback Method
dvisc	0.0000227	Pa×s	900.79	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=U369655&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