Diethylmalonic acid, pentyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C25H32O5/c1-4-7-11-17-28-23(26)25(5-2,6-3)24(27)29-19-20-13-12-16-22(18-

InchiKey: WGQMJCWVCDVGSC-UHFFFAOYSA-N

Formula: C25H32O5

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 412.52

Physical Properties

Property code	Value	Unit	Source
gf	-195.19	kJ/mol	Joback Method
hf	-728.31	kJ/mol	Joback Method
hfus	47.55	kJ/mol	Joback Method
hvap	95.88	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.062		Crippen Method
mcvol	336.340	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	2793.00		NIST Webbook
tb	1001.51	K	Joback Method
tc	1231.22	K	Joback Method
tf	605.84	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.59	J/mol×K	1001.51	Joback Method
cpg	1118.37	J/mol×K	1039.79	Joback Method
cpg	1130.67	J/mol×K	1078.08	Joback Method
cpg	1141.56	J/mol×K	1116.36	Joback Method
cpg	1151.12	J/mol×K	1154.65	Joback Method
cpg	1159.40	J/mol×K	1192.93	Joback Method
cpg	1166.47	J/mol×K	1231.22	Joback Method
dvisc	0.0001796	Pa×s	605.84	Joback Method
dvisc	0.0000974	Pa×s	671.79	Joback Method

dvisc	0.0000589	Pa×s	737.73	Joback Method
dvisc	0.0000387	Pa×s	803.67	Joback Method
dvisc	0.0000271	Pa×s	869.62	Joback Method
dvisc	0.0000199	Pa×s	935.57	Joback Method
dvisc	0.0000153	Pa×s	1001.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370233&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