Diethylmalonic acid, heptyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C27H36O5/c1-4-7-8-9-13-19-30-25(28)27(5-2,6-3)26(29)31-21-22-15-14-18-24

InchiKey: YRRZRWXJOUZZRM-UHFFFAOYSA-N

Formula: C27H36O5

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

Mol. weight [g/mol]: 440.57

Physical Properties

Property code	Value	Unit	Source
gf	-178.35	kJ/mol	Joback Method
hf	-769.59	kJ/mol	Joback Method
hfus	52.73	kJ/mol	Joback Method
hvap	100.34	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.842		Crippen Method
mcvol	364.520	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	3000.00		NIST Webbook
tb	1047.27	K	Joback Method
tc	1282.80	K	Joback Method
tf	628.38	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.06	J/mol×K	1047.27	Joback Method
cpg	1280.48	J/mol×K	1243.54	Joback Method
cpg	1272.39	J/mol×K	1204.29	Joback Method
cpg	1262.98	J/mol×K	1165.03	Joback Method
cpg	1252.18	J/mol×K	1125.78	Joback Method
cpg	1239.90	J/mol×K	1086.52	Joback Method
cpg	1287.34	J/mol×K	1282.80	Joback Method
dvisc	0.0000111	Pa×s	1047.27	Joback Method
dvisc	0.0000146	Pa×s	977.45	Joback Method

dvisc	0.0000199	Pa×s	907.64	Joback Method
dvisc	0.0000287	Pa×s	837.83	Joback Method
dvisc	0.0000441	Pa×s	768.01	Joback Method
dvisc	0.0000739	Pa×s	698.19	Joback Method
dvisc	0.0001390	Pa×s	628.38	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=U370235&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