Diethylmalonic acid, hexyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C26H34O5/c1-4-7-8-12-18-29-24(27)26(5-2,6-3)25(28)30-20-21-14-13-17-23(1

InchiKey: PBHPRZHXPIQMDK-UHFFFAOYSA-N

Formula: C26H34O5

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

Mol. weight [g/mol]: 426.55

Physical Properties

Property code	Value	Unit	Source
gf	-186.77	kJ/mol	Joback Method
hf	-748.95	kJ/mol	Joback Method
hfus	50.14	kJ/mol	Joback Method
hvap	98.11	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.452		Crippen Method
mcvol	350.430	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	2894.00		NIST Webbook
rinpol	2894.00		NIST Webbook
tb	1024.39	K	Joback Method
tc	1256.50	K	Joback Method
tf	617.11	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.12	J/mol×K	1024.39	Joback Method
cpg	1219.73	J/mol×K	1217.82	Joback Method
cpg	1211.54	J/mol×K	1179.13	Joback Method
cpg	1202.05	J/mol×K	1140.45	Joback Method
cpg	1191.21	J/mol×K	1101.76	Joback Method
cpg	1178.92	J/mol×K	1063.08	Joback Method
cpg	1226.70	J/mol×K	1256.50	Joback Method
dvisc	0.0000130	Pa×s	1024.39	Joback Method

dvisc	0.0000171	Pa×s	956.51	Joback Method
dvisc	0.0000232	Pa×s	888.63	Joback Method
dvisc	0.0000333	Pa×s	820.75	Joback Method
dvisc	0.0000510	Pa×s	752.87	Joback Method
dvisc	0.0000849	Pa×s	684.99	Joback Method
dvisc	0.0001582	Pa×s	617.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370234&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