Diethylmalonic acid, octyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C28H38O5/c1-4-7-8-9-10-14-20-31-26(29)28(5-2,6-3)27(30)32-22-23-16-15-19

InchiKey: NISSBEZXEKFNNE-UHFFFAOYSA-N

Formula: C28H38O5

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

Mol. weight [g/mol]: 454.60

Physical Properties

Property code	Value	Unit	Source
gf	-169.93	kJ/mol	Joback Method
hf	-790.23	kJ/mol	Joback Method
hfus	55.32	kJ/mol	Joback Method
hvap	102.56	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.232		Crippen Method
mcvol	378.610	ml/mol	McGowan Method
pc	998.28	kPa	Joback Method
rinpol	3096.00		NIST Webbook
tb	1070.15	K	Joback Method
tc	1310.17	K	Joback Method
tf	639.65	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.36	J/mol×K	1070.15	Joback Method
cpg	1301.26	J/mol×K	1110.15	Joback Method
cpg	1313.56	J/mol×K	1150.16	Joback Method
cpg	1324.32	J/mol×K	1190.16	Joback Method
cpg	1333.65	J/mol×K	1230.16	Joback Method
cpg	1341.64	J/mol×K	1270.16	Joback Method
cpg	1348.38	J/mol×K	1310.17	Joback Method
dvisc	0.0001219	Pa×s	639.65	Joback Method
dvisc	0.0000642	Pa×s	711.40	Joback Method

dvisc	0.0000381	Pa×s	783.15	Joback Method
dvisc	0.0000246	Pa×s	854.90	Joback Method
dvisc	0.0000170	Pa×s	926.65	Joback Method
dvisc	0.0000124	Pa×s	998.40	Joback Method
dvisc	0.0000095	Pa×s	1070.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370236&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