Phthalic acid, 3-methoxybenzyl undecyl ester

Inchi: InChI=1S/C27H36O5/c1-3-4-5-6-7-8-9-10-13-19-31-26(28)24-17-11-12-18-25(24)27(29)3
InchiKey: PAISZXYDNULBRJ-UHFFFAOYSA-N
Formula: C27H36O5
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(OC)c1
Mol. weight [g/mol]: 440.57

Physical Properties

Property code	Value	Unit	Source
gf	-190.82	kJ/mol	Joback Method
hf	-772.31	kJ/mol	Joback Method
hfus	59.75	kJ/mol	Joback Method
hvap	102.29	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	6.740		Crippen Method
mcvol	364.520	ml/mol	McGowan Method
pc	1038.57	kPa	Joback Method
rinpol	3306.00		NIST Webbook
tb	1055.48	K	Joback Method
tc	1292.22	K	Joback Method
tf	638.48	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.51	J/mol×K	1055.48	Joback Method
cpg	1237.79	J/mol×K	1094.94	Joback Method
cpg	1249.26	J/mol×K	1134.39	Joback Method
cpg	1258.98	J/mol×K	1173.85	Joback Method
cpg	1266.99	J/mol×K	1213.30	Joback Method
cpg	1273.33	J/mol×K	1252.76	Joback Method
cpg	1278.06	J/mol×K	1292.22	Joback Method
dvisc	0.0001492	Pa×s	638.48	Joback Method
dvisc	0.0000848	Pa×s	707.98	Joback Method

dvisc	0.0000533	Pa×s	777.48	Joback Method
dvisc	0.0000362	Pa×s	846.98	Joback Method
dvisc	0.0000260	Pa×s	916.48	Joback Method
dvisc	0.0000196	Pa×s	985.98	Joback Method
dvisc	0.0000154	Pa×s	1055.48	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=U377984&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