Phthalic acid, 3-methoxybenzyl octyl ester

Inchi: InChI=1S/C24H30O5/c1-3-4-5-6-7-10-16-28-23(25)21-14-8-9-15-22(21)24(26)29-18-19-1
InchiKey: GOZOCKQDMYCCFO-UHFFFAOYSA-N
Formula: C24H30O5
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(OC)c1
Mol. weight [g/mol]: 398.49

Physical Properties

Property code	Value	Unit	Source
gf	-216.08	kJ/mol	Joback Method
hf	-710.39	kJ/mol	Joback Method
hfus	51.98	kJ/mol	Joback Method
hvap	95.62	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	5.569		Crippen Method
mcvol	322.250	ml/mol	McGowan Method
pc	1261.95	kPa	Joback Method
rinpol	3002.00		NIST Webbook
rinpol	3002.00		NIST Webbook
tb	986.84	K	Joback Method
tc	1212.48	K	Joback Method
tf	604.67	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.07	J/mol×K	986.84	Joback Method
cpg	1094.47	J/mol×K	1174.87	Joback Method
cpg	1087.20	J/mol×K	1137.27	Joback Method
cpg	1078.46	J/mol×K	1099.66	Joback Method
cpg	1068.21	J/mol×K	1062.05	Joback Method
cpg	1056.42	J/mol×K	1024.45	Joback Method
cpg	1100.29	J/mol×K	1212.48	Joback Method
dvisc	0.0000241	Pa×s	986.84	Joback Method

dvisc	0.0000306	Pa×s	923.14	Joback Method
dvisc	0.0000402	Pa×s	859.45	Joback Method
dvisc	0.0000551	Pa×s	795.75	Joback Method
dvisc	0.0000799	Pa×s	732.06	Joback Method
dvisc	0.0001242	Pa×s	668.37	Joback Method
dvisc	0.0002121	Pa×s	604.67	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U377981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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