

Phthalic acid, 3-methoxybenzyl tetradecyl ester

Inchi: InChI=1S/C30H42O5/c1-3-4-5-6-7-8-9-10-11-12-13-16-22-34-29(31)27-20-14-15-21-28(2)
InchiKey: OBGWIAUIAJTHLQ-UHFFFAOYSA-N
Formula: C30H42O5
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(OC)c1
Mol. weight [g/mol]: 482.65

Physical Properties

Property code	Value	Unit	Source
gf	-165.56	kJ/mol	Joback Method
hf	-834.23	kJ/mol	Joback Method
hfus	67.52	kJ/mol	Joback Method
hvap	108.97	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	7.910		Crippen Method
mcvol	406.790	ml/mol	McGowan Method
pc	869.65	kPa	Joback Method
rinpol	3605.00		NIST Webbook
tb	1124.12	K	Joback Method
tc	1382.23	K	Joback Method
tf	672.29	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1408.58	J/mol×K	1124.12	Joback Method
cpg	1453.65	J/mol×K	1339.21	Joback Method
cpg	1448.69	J/mol×K	1296.19	Joback Method
cpg	1441.78	J/mol×K	1253.17	Joback Method
cpg	1432.84	J/mol×K	1210.16	Joback Method
cpg	1421.80	J/mol×K	1167.14	Joback Method
cpg	1456.74	J/mol×K	1382.23	Joback Method
dvisc	0.0000096	Pa×s	1124.12	Joback Method
dvisc	0.0000124	Pa×s	1048.81	Joback Method

dvisc	0.0000166	Pa×s	973.51	Joback Method
dvisc	0.0000233	Pa×s	898.20	Joback Method
dvisc	0.0000349	Pa×s	822.90	Joback Method
dvisc	0.0000567	Pa×s	747.60	Joback Method
dvisc	0.0001026	Pa×s	672.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377987&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

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