Phthalic acid, hexadecyl 3-methoxybenzyl ester

Inchi: InChI=1S/C32H46O5/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-24-36-31(33)29-22-16-17-2

InchiKey: LQIJQAIFTQHRPS-UHFFFAOYSA-N

Formula: C32H46O5

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(OC)c1

Mol. weight [g/mol]: 510.70

Physical Properties

Property code	Value	Unit	Source
gf	-148.72	kJ/mol	Joback Method
hf	-875.51	kJ/mol	Joback Method
hfus	72.70	kJ/mol	Joback Method
hvap	113.42	kJ/mol	Joback Method
log10ws	-10.47		Crippen Method
logp	8.690		Crippen Method
mcvol	434.970	ml/mol	McGowan Method
pc	778.94	kPa	Joback Method
rinpol	3809.00		NIST Webbook
tb	1169.88	K	Joback Method
tc	1449.06	K	Joback Method
tf	694.83	K	Joback Method
vc	1.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1532.23	J/mol×K	1169.88	Joback Method
cpg	1573.87	J/mol×K	1402.53	Joback Method
cpg	1570.18	J/mol×K	1356.00	Joback Method
cpg	1564.28	J/mol×K	1309.47	Joback Method
cpg	1556.07	J/mol×K	1262.94	Joback Method
cpg	1545.42	J/mol×K	1216.41	Joback Method
cpg	1575.48	J/mol×K	1449.06	Joback Method
dvisc	0.0000070	Pa×s	1169.88	Joback Method
dvisc	0.0000091	Pa×s	1090.71	Joback Method

dvisc	0.0000122	Pa×s	1011.53	Joback Method
dvisc	0.0000173	Pa×s	932.36	Joback Method
dvisc	0.0000261	Pa×s	853.18	Joback Method
dvisc	0.0000429	Pa×s	774.01	Joback Method
dvisc	0.0000790	Pa×s	694.83	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=U377989&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