

Phthalic acid, 3-methoxybenzyl pentadecyl ester

Inchi:	InChI=1S/C31H44O5/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-23-35-30(32)28-21-15-16-22-2
InchiKey:	VJPUBWYHAORFMA-UHFFFAOYSA-N
Formula:	C31H44O5
SMILES:	CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(OC)c1
Mol. weight [g/mol]:	496.68

Physical Properties

Property code	Value	Unit	Source
gf	-157.14	kJ/mol	Joback Method
hf	-854.87	kJ/mol	Joback Method
hfus	70.11	kJ/mol	Joback Method
hvap	111.20	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	8.300		Crippen Method
mvol	420.880	ml/mol	McGowan Method
pc	822.42	kPa	Joback Method
rinpol	3707.00		NIST Webbook
rinpol	3707.00		NIST Webbook
tb	1147.00	K	Joback Method
tc	1414.90	K	Joback Method
tf	683.56	K	Joback Method
vc	1.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1470.33	J/molxK	1147.00	Joback Method
cpg	1483.54	J/molxK	1191.65	Joback Method
cpg	1494.40	J/molxK	1236.30	Joback Method
cpg	1503.00	J/molxK	1280.95	Joback Method
cpg	1509.43	J/molxK	1325.60	Joback Method
cpg	1513.80	J/molxK	1370.25	Joback Method
cpg	1516.19	J/molxK	1414.90	Joback Method
dvisc	0.0000901	Paxs	683.56	Joback Method

dvisc	0.0000493	Paxs	760.80	Joback Method
dvisc	0.0000302	Paxs	838.04	Joback Method
dvisc	0.0000201	Paxs	915.28	Joback Method
dvisc	0.0000142	Paxs	992.52	Joback Method
dvisc	0.0000106	Paxs	1069.76	Joback Method
dvisc	0.0000082	Paxs	1147.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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