

Hexadecyl methyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, hexadecyl methyl ester Phthalic acid, hexadecyl methyl ester
Inchi:	InChI=1S/C25H40O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-29-25(27)23-20-17-16-1
InchiKey:	CPCNZWLOGJACQU-UHFFFAOYSA-N
Formula:	C25H40O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC
Mol. weight [g/mol]:	404.58
CAS:	101762-77-0

Physical Properties

Property code	Value	Unit	Source
gf	-205.44	kJ/mol	Joback Method
hf	-823.87	kJ/mol	Joback Method
hfus	59.73	kJ/mol	Joback Method
hvap	92.49	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.111		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	970.49	kPa	Joback Method
rinpol	2962.00		NIST Webbook
tb	955.64	K	Joback Method
tc	1169.97	K	Joback Method
tf	554.77	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.32	J/mol×K	955.64	Joback Method
cpg	1198.61	J/mol×K	991.36	Joback Method
cpg	1214.46	J/mol×K	1027.08	Joback Method
cpg	1228.89	J/mol×K	1062.81	Joback Method
cpg	1241.97	J/mol×K	1098.53	Joback Method
cpg	1253.73	J/mol×K	1134.25	Joback Method

cpg	1264.21	J/mol×K	1169.97	Joback Method
dvisc	0.0003423	Pa×s	554.77	Joback Method
dvisc	0.0001777	Pa×s	621.58	Joback Method
dvisc	0.0001048	Pa×s	688.39	Joback Method
dvisc	0.0000678	Pa×s	755.20	Joback Method
dvisc	0.0000471	Pa×s	822.02	Joback Method
dvisc	0.0000346	Pa×s	888.83	Joback Method
dvisc	0.0000265	Pa×s	955.64	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=C101762770&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/27-340-4/Hexadecyl-methyl-phthalate.pdf>

Generated by Cheméo on 2025-12-05 16:10:14.166724263 +0000 UTC m=+4699211.696764918.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.