Phthalic acid, hexadecyl methyl ester

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]: 404.59

Physical Properties

Property code	Value	Unit	Source
af	1.1863		Cheméo Relay (1.0)
hf	-914.95	kJ/mol	Cheméo Relay (1.0)
hfus	59.73	kJ/mol	Joback Method
hvap	122.30	kJ/mol	Cheméo Relay (1.0)
ie	9.43	eV	Cheméo Relay (1.0)
log10ws	-7.42		Cheméo Relay (1.0)
logp	7.111		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	970.49	kPa	Joback Method
rinpol	2962.00		NIST Webbook
tb	662.04	K	Cheméo Relay (1.0)
tc	871.41	K	Cheméo Relay (1.0)
tf	300.66	K	Cheméo Relay (1.0)
vc	1.348	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.32	J/mol×K	955.64	Joback Method
cpg	1264.21	J/mol×K	1169.97	Joback Method
cpg	1253.73	J/mol×K	1134.25	Joback Method
cpg	1241.97	J/mol×K	1098.53	Joback Method
cpg	1228.89	J/mol×K	1062.81	Joback Method
cpg	1214.46	J/mol×K	1027.08	Joback Method

cpg	1198.61	J/mol×K	991.36	Joback Method
dvisc	0.0000678	Pa×s	755.20	Joback Method
dvisc	0.0000265	Pa×s	955.64	Joback Method
dvisc	0.0000346	Pa×s	888.83	Joback Method
dvisc	0.0000471	Pa×s	822.02	Joback Method
dvisc	0.0003423	Pa×s	554.77	Joback Method
dvisc	0.0001048	Pa×s	688.39	Joback Method
dvisc	0.0001777	Pa×s	621.58	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101762770&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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