Cyclohexyl methyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, cyclohexyl methyl ester
Inchi: InChI=1S/C15H18O4/c1-18-14(16)12-9-5-6-10-13(12)15(17)19-11-7-3-2-4-8-11/h5-6,9-1
InchiKey: PFRYPBLKZWQNCG-UHFFFAOYSA-N
Formula: C15H18O4
SMILES: COC(=O)c1ccccc1C(=O)OC1CCCCC1
Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-265.19	kJ/mol	Joback Method
hf	-563.15	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	70.66	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.963		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	2023.00		NIST Webbook
tb	746.39	K	Joback Method
tc	980.17	K	Joback Method
tf	449.45	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.64	J/mol×K	746.39	Joback Method
cpg	603.50	J/mol×K	785.35	Joback Method
cpg	618.95	J/mol×K	824.32	Joback Method
cpg	633.02	J/mol×K	863.28	Joback Method
cpg	645.74	J/mol×K	902.25	Joback Method
cpg	657.10	J/mol×K	941.21	Joback Method
cpg	667.14	J/mol×K	980.17	Joback Method
dvisc	0.0010726	Pa×s	449.45	Joback Method

dvisc	0.0006089	Pa×s	498.94	Joback Method
dvisc	0.0003828	Pa×s	548.43	Joback Method
dvisc	0.0002599	Pa×s	597.92	Joback Method
dvisc	0.0001872	Pa×s	647.41	Joback Method
dvisc	0.0001413	Pa×s	696.90	Joback Method
dvisc	0.0001107	Pa×s	746.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373813&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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