Phthalic acid, monocyclohexyl ester

Other names:	1,2-Benzenedicarboxylic acid, monocyclohexyl ester
	Cyclohexyl hydrogen phthalate
	Mchp
	Monocyclohexyl phthalate
	2-(Cyclohexyloxycarbonyl)benzoic acid
Inchi:	InChI=1S/C14H16O4/c15-13(16)11-8-4-5-9-12(11)14(17)18-10-6-2-1-3-7-10/h4-5,8-10H,
InchiKey:	PMDKYLLIOLFQPO-UHFFFAOYSA-N
Formula:	C14H16O4
SMILES:	O=C(O)c1ccccc1C(=O)OC1CCCCC1
Mol. weight [g/mol]:	248.27
CAS:	7517-36-4

Physical Properties

Property code	Value	Unit	Source
gf	-305.43	kJ/mol	Joback Method
hf	-562.52	kJ/mol	Joback Method
hfus	25.98	kJ/mol	Joback Method
hvap	82.71	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.874		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
tb	793.27	K	Joback Method
tc	1017.09	K	Joback Method
tf	476.77	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.74	J/mol×K	793.27	Joback Method
cpg	573.99	J/mol×K	830.57	Joback Method

cpg	586.11	J/mol×K	867.88	Joback Method
cpg	597.11	J/mol×K	905.18	Joback Method
cpg	607.04	J/mol×K	942.48	Joback Method
cpg	615.93	J/mol×K	979.79	Joback Method
cpg	623.80	J/mol×K	1017.09	Joback Method
dvisc	0.0008951	Pa×s	476.77	Joback Method
dvisc	0.0003825	Pa×s	529.52	Joback Method
dvisc	0.0001907	Pa×s	582.27	Joback Method
dvisc	0.0001067	Pa×s	635.02	Joback Method
dvisc	0.0000653	Pa×s	687.77	Joback Method
dvisc	0.0000428	Pa×s	740.52	Joback Method
dvisc	0.0000297	Pa×s	793.27	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=C7517364&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