Piperonyl acetate

Other names:	Piperonyl acetate
	1,3-Benzodioxole-5-methanol, acetate
	Acetic acid, (3,4-methylenedioxy)benzyl ester
	Heliotropyl acetate
	Piperonyl alcohol, acetate
	1,3-Benzodioxol, 5-(acetoxymethyl)
	Piperonal acetate
Inchi:	InChI=1S/C10H10O4/c1-7(11)12-5-8-2-3-9-10(4-8)14-6-13-9/h2-4H,5-6H2,1H3
InchiKey:	PFWYHTORQZAGCA-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	CC(=O)OCc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	194.19

Physical Properties

Property code	Value	Unit	Source
hfus	30.73	kJ/mol	Joback Method
hvap	74.31	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-2.58		Cheméo Relay (1.0)
logp	1.478		Crippen Method
mcvol	136.320	ml/mol	McGowan Method
rinpol	1485.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1514.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2344.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2344.00		NIST Webbook
tb	545.29	K	Cheméo Relay (1.0)
tf	297.98	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.90	J/mol×K	606.44	Joback Method
cpg	350.92	J/mol×K	644.16	Joback Method
cpg	362.13	J/mol×K	681.88	Joback Method
cpg	372.58	J/mol×K	719.59	Joback Method
cpg	382.30	J/mol×K	757.31	Joback Method
cpg	391.33	J/mol×K	795.03	Joback Method
cpg	399.73	J/mol×K	832.75	Joback Method
dvisc	0.0017744	Pa×s	401.40	Joback Method
dvisc	0.0012636	Pa×s	435.57	Joback Method
dvisc	0.0009454	Pa×s	469.75	Joback Method
dvisc	0.0007358	Pa×s	503.92	Joback Method
dvisc	0.0005911	Pa×s	538.09	Joback Method
dvisc	0.0004875	Pa×s	572.27	Joback Method
dvisc	0.0004109	Pa×s	606.44	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C326614&Units=SI
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):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point