ISOPENTYL DL-MANDELATE

Other names:	Benzeneacetic acid, «alpha»-hydroxy-, 3-methylbutyl ester
	Atractyl
	Mandaverm
	Mandelic acid isoamyl ester
	Mandelic acid, isopentyl ester
	Spasmol
	Spasmostenyl
	Vermiparin
	Isopentyl alcohol, mandelate
	isopentyl phenylglycolate
Inchi:	InChI=1S/C13H18O3/c1-10(2)8-9-16-13(15)12(14)11-6-4-3-5-7-11/h3-7,10,12,14H,8-9H2
InchiKey:	KQQXUARABJGCMS-UHFFFAOYSA-N
Formula:	C13H18O3
SMILES:	CC(C)CCOC(=O)C(O)c1ccccc1
Mol. weight [g/mol]:	222.28

Physical Properties

Property code	Value	Unit	Source
hf	-567.88	kJ/mol	Cheméo Relay (1.0)
hfus	23.30	kJ/mol	Joback Method
hvap	79.83	kJ/mol	Cheméo Relay (1.0)
ie	8.97	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	2.309		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
tb	549.20	K	Cheméo Relay (1.0)
tc	781.92	K	Cheméo Relay (1.0)
tf	308.51	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.90	J/mol×K	691.11	Joback Method

cpg	516.31	J/mol×K	724.17	Joback Method
cpg	528.91	J/mol×K	757.22	Joback Method
cpg	540.72	J/mol×K	790.28	Joback Method
cpg	551.76	J/mol×K	823.34	Joback Method
cpg	562.05	J/mol×K	856.40	Joback Method
cpg	571.63	J/mol×K	889.45	Joback Method
dvisc	0.0043108	Pa×s	365.67	Joback Method
dvisc	0.0011538	Pa×s	419.91	Joback Method
dvisc	0.0004175	Pa×s	474.15	Joback Method
dvisc	0.0001861	Pa×s	528.39	Joback Method
dvisc	0.0000964	Pa×s	582.63	Joback Method
dvisc	0.0000559	Pa×s	636.87	Joback Method
dvisc	0.0000353	Pa×s	691.11	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5421045&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):

Legend

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point