

Methyl 3-(4-hydroxy-3-methoxyphenyl)propanoate

Inchi: InChI=1S/C11H14O4/c1-14-10-7-8(3-5-9(10)12)4-6-11(13)15-2/h3,5,7,12H,4,6H2,1-2H3
InchiKey: PDTCYIZPTRRYOT-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: COC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
hf	-635.67	kJ/mol	Cheméo Relay (1.0)
hfus	27.66	kJ/mol	Joback Method
hvap	90.98	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-1.90		Cheméo Relay (1.0)
logp	1.506		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
rinpol	1644.00		NIST Webbook
rinpol	1683.80		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1683.80		NIST Webbook
tb	567.26	K	Cheméo Relay (1.0)
tf	325.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.72	J/mol×K	662.07	Joback Method
cpg	434.18	J/mol×K	698.34	Joback Method
cpg	445.92	J/mol×K	734.62	Joback Method
cpg	456.99	J/mol×K	770.89	Joback Method
cpg	467.41	J/mol×K	807.17	Joback Method
cpg	477.24	J/mol×K	843.44	Joback Method
cpg	486.51	J/mol×K	879.72	Joback Method
dvisc	0.0003177	Pa×s	458.78	Joback Method
dvisc	0.0001660	Pa×s	492.66	Joback Method

dvisc	0.0000943	Pa×s	526.54	Joback Method
dvisc	0.0000573	Pa×s	560.43	Joback Method
dvisc	0.0000369	Pa×s	594.31	Joback Method
dvisc	0.0000249	Pa×s	628.19	Joback Method
dvisc	0.0000175	Pa×s	662.07	Joback Method

Sources

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=C56024443&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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