

ethyl 4-methoxy-6-methylsalicylate

Other names:	Ethyl 2-hydroxy-4-methoxy-6-methylbenzoate
Inchi:	InChI=1S/C11H14O4/c1-4-15-11(13)10-7(2)5-8(14-3)6-9(10)12/h5-6,12H,4H2,1-3H3
InchiKey:	PJOOIAZRUIIQMU-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	CCOC(=O)c1c(C)cc(OC)cc1O
Mol. weight [g/mol]:	210.23
CAS:	6110-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-358.65	kJ/mol	Joback Method
hf	-611.11	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	68.26	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.886		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1680.10		NIST Webbook
rinpol	1680.10		NIST Webbook
tb	667.05	K	Joback Method
tc	885.56	K	Joback Method
tf	471.30	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.53	J/molxK	667.05	Joback Method
cpg	432.84	J/molxK	703.47	Joback Method
cpg	444.47	J/molxK	739.89	Joback Method
cpg	455.46	J/molxK	776.31	Joback Method
cpg	465.83	J/molxK	812.72	Joback Method
cpg	475.62	J/molxK	849.14	Joback Method

cpg	484.86	J/molxK	885.56	Joback Method
dvisc	0.0002436	Paxs	471.30	Joback Method
dvisc	0.0001353	Paxs	503.93	Joback Method
dvisc	0.0000807	Paxs	536.55	Joback Method
dvisc	0.0000511	Paxs	569.17	Joback Method
dvisc	0.0000340	Paxs	601.80	Joback Method
dvisc	0.0000236	Paxs	634.42	Joback Method
dvisc	0.0000170	Paxs	667.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6110367&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

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