

(.+/-.)-Tremetone

Inchi:	InChI=1S/C13H14O2/c1-8(2)13-7-11-6-10(9(3)14)4-5-12(11)15-13/h4-6,13H,1,7H2,2-3H
InchiKey:	UVYUUQGGBNKRUFU-UHFFFAOYSA-N
Formula:	C13H14O2
SMILES:	<chem>C=C(C)C1Cc2cc(C(C)=O)ccc2O1</chem>
Mol. weight [g/mol]:	202.25
CAS:	59183-49-2

Physical Properties

Property code	Value	Unit	Source
gf	76.73	kJ/mol	Joback Method
hf	-154.20	kJ/mol	Joback Method
hfus	27.81	kJ/mol	Joback Method
hvap	58.71	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.769		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1746.70		NIST Webbook
rinpol	1746.70		NIST Webbook
tb	617.60	K	Joback Method
tc	845.46	K	Joback Method
tf	366.45	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.26	J/molxK	617.60	Joback Method
cpg	426.38	J/molxK	655.58	Joback Method
cpg	440.47	J/molxK	693.55	Joback Method
cpg	453.58	J/molxK	731.53	Joback Method
cpg	465.80	J/molxK	769.51	Joback Method
cpg	477.19	J/molxK	807.49	Joback Method
cpg	487.83	J/molxK	845.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C59183492&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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