

Tasmanone

Inchi:	InChI=1S/C14H20O4/c1-7(2)10(15)9-11(16)8(3)13(18-6)14(4,5)12(9)17/h7,9H,1-6H3
InchiKey:	WZXQWLWGLWIQGK-UHFFFAOYSA-N
Formula:	C14H20O4
SMILES:	COC1=C(C)C(=O)C(C(=O)C(C)C)C(=O)C1(C)C
Mol. weight [g/mol]:	252.31
CAS:	22595-52-4

Physical Properties

Property code	Value	Unit	Source
gf	-392.59	kJ/mol	Joback Method
hf	-773.71	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	64.61	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.926		Crippen Method
mcvol	203.540	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
ripol	2288.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2288.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2303.00		NIST Webbook
tb	755.45	K	Joback Method
tc	985.94	K	Joback Method
tf	493.98	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.91	J/mol×K	755.45	Joback Method
cpg	626.12	J/mol×K	793.86	Joback Method
cpg	643.45	J/mol×K	832.28	Joback Method
cpg	659.93	J/mol×K	870.69	Joback Method
cpg	675.59	J/mol×K	909.11	Joback Method
cpg	690.47	J/mol×K	947.52	Joback Method
cpg	704.61	J/mol×K	985.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22595524&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

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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