

3-Oxabicyclo[3.2.1]octane-2,4-dione, 1,8,8-trimethyl-, (1S)-

Other names:	(1S)-1,8,8-trimethyl-3-oxabicyclo[3.2.1]octane-2,4-dione (d)-camphoric anhydride
Inchi:	InChI=1S/C10H14O3/c1-9(2)6-4-5-10(9,3)8(12)13-7(6)11/h6H,4-5H2,1-3H3
InchiKey:	VFZDNKRDYPTSTP-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CC12CCC(C(=O)OC1=O)C2(C)C
Mol. weight [g/mol]:	182.22
CAS:	595-31-3

Physical Properties

Property code	Value	Unit	Source
gf	-219.37	kJ/mol	Joback Method
hf	-513.71	kJ/mol	Joback Method
hfus	9.20	kJ/mol	Joback Method
hvap	48.42	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.512		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	608.62	K	Joback Method
tc	862.17	K	Joback Method
tf	437.87	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.72	J/mol×K	777.65	Joback Method
cpg	466.20	J/mol×K	819.91	Joback Method
cpg	385.35	J/mol×K	608.62	Joback Method
cpg	402.73	J/mol×K	650.88	Joback Method
cpg	419.25	J/mol×K	693.14	Joback Method
cpg	435.16	J/mol×K	735.39	Joback Method
cpg	481.85	J/mol×K	862.17	Joback Method

hfust	5.65	kJ/mol	493.60	NIST Webbook
hfust	8.70	kJ/mol	495.00	NIST Webbook

Sources

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=C595313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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