Acorone

Inchi: InChI=1S/C15H24O2/c1-9(2)14-12(16)7-11(4)15(14)6-5-10(3)13(17)8-15/h9-11,14H,5-8H
InchiKey: AGUISGUERLMHFF-VIQGCOBNSA-N
Formula: C15H24O2
SMILES: CC1CCC2(CC1=O)C(C)CC(=O)C2C(C)C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-120.01	kJ/mol	Joback Method
hf	-538.09	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	55.83	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.243		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	699.26	K	Joback Method
tc	941.42	K	Joback Method
tf	417.47	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.74	J/mol×K	699.26	Joback Method
cpg	652.57	J/mol×K	739.62	Joback Method
cpg	675.10	J/mol×K	779.98	Joback Method
cpg	696.41	J/mol×K	820.34	Joback Method
cpg	716.60	J/mol×K	860.70	Joback Method
cpg	735.80	J/mol×K	901.06	Joback Method
cpg	754.08	J/mol×K	941.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R275240&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
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