2-Acetyl-1,3-cyclohexanedione

Other names: 1,3-Cyclohexanedione, 2-acetyl-
Inchi: InChI=1S/C8H10O3/c1-5(9)8-6(10)3-2-4-7(8)11/h8H,2-4H2,1H3
InchiKey: CHNXDYRMRBQOEF-UHFFFAOYSA-N
Formula: C8H10O3
SMILES: CC(=O)C1C(=O)CCCC1=O
Mol. weight [g/mol]: 154.16
CAS: 4056-73-9

Physical Properties

Property code	Value	Unit	Source
gf	-333.17	kJ/mol	Joback Method
hf	-542.11	kJ/mol	Joback Method
hfus	8.93	kJ/mol	Joback Method
hvap	49.07	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	0.514		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	591.50	K	Joback Method
tc	836.66	K	Joback Method
tf	303.50 ± 1.50	K	NIST Webbook
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.32	J/mol×K	591.50	Joback Method
cpg	309.84	J/mol×K	632.36	Joback Method
cpg	324.52	J/mol×K	673.22	Joback Method
cpg	338.28	J/mol×K	714.08	Joback Method
cpg	351.09	J/mol×K	754.94	Joback Method
cpg	362.87	J/mol×K	795.80	Joback Method
cpg	373.57	J/mol×K	836.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.70	K	2.90	NIST Webbook
tbrp	399.50 ± 0.50	K	2.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4056739&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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