2,4-Heptanedione, 6-methyl-

Other names:	6-Methyl-2,4-heptanedione
	6-Methylheptan-2,4-dione
	6-Methylheptane-2,4-dione
	6-methyl-2,4-heptadione
Inchi:	InChI=1S/C8H14O2/c1-6(2)4-8(10)5-7(3)9/h6H,4-5H2,1-3H3
InchiKey:	IGMOYJSFRIASIE-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC(=O)CC(=O)CC(C)C
Mol. weight [g/mol]:	142.20
CAS:	3002-23-1

Physical Properties

Property code	Value	Unit	Source
gf	-243.80	kJ/mol	Joback Method
hf	-456.50	kJ/mol	NIST Webbook
hfus	16.15	kJ/mol	Joback Method
hvap	46.51	kJ/mol	Joback Method
log10ws	-1.60		Aqueous Solubility Prediction Method
logp	1.581		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1000.00		NIST Webbook
rinpol	1033.26		NIST Webbook
rinpol	1036.02		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1028.70		NIST Webbook
rinpol	1032.09		NIST Webbook
tb	489.74	K	Joback Method
tc	679.53	K	Joback Method
tf	264.78	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.42	J/mol×K	489.74	Joback Method
cpg	287.52	J/mol×K	521.37	Joback Method
cpg	299.07	J/mol×K	553.00	Joback Method
cpg	310.09	J/mol×K	584.63	Joback Method
cpg	320.57	J/mol×K	616.27	Joback Method
cpg	330.55	J/mol×K	647.90	Joback Method
cpg	340.02	J/mol×K	679.53	Joback Method
dvisc	0.0050267	Pa×s	264.78	Joback Method
dvisc	0.0023823	Pa×s	302.27	Joback Method
dvisc	0.0013314	Pa×s	339.77	Joback Method
dvisc	0.0008352	Pa×s	377.26	Joback Method
dvisc	0.0005701	Pa×s	414.75	Joback Method
dvisc	0.0004145	Pa×s	452.25	Joback Method
dvisc	0.0003165	Pa×s	489.74	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3002231&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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