3-n-Propyl-2,4-pentanedione

Other names:	2,4-Pentanedione, 3-propyl-
	3-Propylacetylacetone
	3-propyl-2,4-pentadione
	3-propylpentane-2,4-dione
Inchi:	InChI=1S/C8H14O2/c1-4-5-8(6(2)9)7(3)10/h8H,4-5H2,1-3H3
InchiKey:	AQGSZYZZVTYOMQ-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CCCC(C(C)=O)C(C)=O
Mol. weight [g/mol]:	142.20
CAS:	1540-35-8

Physical Properties

Property code	Value	Unit	Source
gf	-243.80	kJ/mol	Joback Method
hf	-453.10	kJ/mol	NIST Webbook
hfus	16.15	kJ/mol	Joback Method
hvap	46.51	kJ/mol	Joback Method
log10ws	-0.88		Aqueous Solubility Prediction Method
logp	1.581		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
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	330.55	J/mol×K	647.90	Joback Method
cpg	320.57	J/mol×K	616.27	Joback Method
cpg	310.09	J/mol×K	584.63	Joback Method

cpg	299.07	J/mol×K	553.00	Joback Method
cpg	287.52	J/mol×K	521.37	Joback Method
cpg	340.02	J/mol×K	679.53	Joback Method
dvisc	0.0003165	Pa×s	489.74	Joback Method
dvisc	0.0004145	Pa×s	452.25	Joback Method
dvisc	0.0005701	Pa×s	414.75	Joback Method
dvisc	0.0008352	Pa×s	377.26	Joback Method
dvisc	0.0013314	Pa×s	339.77	Joback Method
dvisc	0.0023823	Pa×s	302.27	Joback Method
dvisc	0.0050267	Pa×s	264.78	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1540358&Units=SI

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