

2,4-Pentanedione, 3-(2-propenyl)-

Other names:	2,4-Pentanedione, 3-allyl- 3-Allyl-2,4-pentanedione 3-Allylacetylacetone 2-Allyl-1-mehtylbutandione-1,3
Inchi:	InChI=1S/C8H12O2/c1-4-5-8(6(2)9)7(3)10/h4,8H,1,5H2,2-3H3
InchiKey:	QBQVCCUJHAORJO-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	C=CCC(C(C)=O)C(C)=O
Mol. weight [g/mol]:	140.18
CAS:	3508-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-155.96	kJ/mol	Joback Method
hf	-313.46	kJ/mol	Joback Method
hfus	14.87	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.357		Crippen Method
mcvol	122.420	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	472.20	K	NIST Webbook
tc	680.14	K	Joback Method
tf	263.02	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.98	J/molxK	486.42	Joback Method
cpg	269.42	J/molxK	518.71	Joback Method
cpg	280.29	J/molxK	550.99	Joback Method
cpg	290.62	J/molxK	583.28	Joback Method
cpg	300.42	J/molxK	615.57	Joback Method

cpg	309.70	J/molxK	647.86	Joback Method
cpg	318.48	J/molxK	680.14	Joback Method
dvisc	0.0046183	Paxs	263.02	Joback Method
dvisc	0.0022463	Paxs	300.25	Joback Method
dvisc	0.0012809	Paxs	337.49	Joback Method
dvisc	0.0008166	Paxs	374.72	Joback Method
dvisc	0.0005648	Paxs	411.95	Joback Method
dvisc	0.0004152	Paxs	449.19	Joback Method
dvisc	0.0003200	Paxs	486.42	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.20	K	2.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3508789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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