

2,4-Nonanedione

Other names:	nonane-2,4-dione
Inchi:	InChI=1S/C9H16O2/c1-3-4-5-6-9(11)7-8(2)10/h3-7H2,1-2H3
InchiKey:	KFBXUKHERGLHLG-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CCCCC(=O)CC(C)=O
Mol. weight [g/mol]:	156.22
CAS:	6175-23-1

Physical Properties

Property code	Value	Unit	Source
gf	-232.94	kJ/mol	Joback Method
hf	-454.25	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.115		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1136.19		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1152.00		NIST Webbook
tb	513.06	K	Joback Method
tc	696.84	K	Joback Method
tf	291.05	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.07	J/molxK	513.06	Joback Method
cpg	331.79	J/molxK	543.69	Joback Method
cpg	343.95	J/molxK	574.32	Joback Method
cpg	355.55	J/molxK	604.95	Joback Method
cpg	366.62	J/molxK	635.58	Joback Method

cpg	377.16	J/mol×K	666.21	Joback Method
cpg	387.18	J/mol×K	696.84	Joback Method
dvisc	0.0036476	Paxs	291.05	Joback Method
dvisc	0.0019243	Paxs	328.05	Joback Method
dvisc	0.0011556	Paxs	365.05	Joback Method
dvisc	0.0007623	Paxs	402.05	Joback Method
dvisc	0.0005394	Paxs	439.06	Joback Method
dvisc	0.0004027	Paxs	476.06	Joback Method
dvisc	0.0003137	Paxs	513.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37887e+01
Coeff. B	-3.78178e+03
Coeff. C	-7.12340e+01
Temperature range (K), min.	351.34
Temperature range (K), max.	517.34

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6175231&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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