

3-methylnonane-2,4-dione

Other names:	2,4-Nonanedione, 3-methyl 3-methyl-2,4-nonanedione 3-methyl-2,4-nonandione 3-Methyl-2,4-nonadione
Inchi:	InChI=1S/C10H18O2/c1-4-5-6-7-10(12)8(2)9(3)11/h8H,4-7H2,1-3H3
InchiKey:	BGVBGAIWXAXBLP-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CCCCC(=O)C(C)C(C)=O
Mol. weight [g/mol]:	170.25
CAS:	113486-29-6

Physical Properties

Property code	Value	Unit	Source
gf	-226.96	kJ/mol	Joback Method
hf	-480.17	kJ/mol	Joback Method
hfus	21.33	kJ/mol	Joback Method
hvap	50.96	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.361		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1253.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1253.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1722.00		NIST Webbook

ripol	1723.00		NIST Webbook
ripol	1715.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1726.00		NIST Webbook
tb	535.50	K	Joback Method
tc	721.00	K	Joback Method
tf	287.32	K	Joback Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.13	J/mol×K	535.50	Joback Method
cpg	428.38	J/mol×K	690.09	Joback Method
cpg	416.95	J/mol×K	659.17	Joback Method
cpg	404.92	J/mol×K	628.25	Joback Method
cpg	392.29	J/mol×K	597.33	Joback Method
cpg	379.03	J/mol×K	566.42	Joback Method
cpg	439.24	J/mol×K	721.00	Joback Method
dvisc	0.0002740	Pa×s	535.50	Joback Method
dvisc	0.0003620	Pa×s	494.14	Joback Method
dvisc	0.0005032	Pa×s	452.77	Joback Method
dvisc	0.0007476	Pa×s	411.41	Joback Method
dvisc	0.0012132	Pa×s	370.05	Joback Method
dvisc	0.0022242	Pa×s	328.68	Joback Method
dvisc	0.0048550	Pa×s	287.32	Joback Method

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>

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

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