

2,11-Dodecanedione

Inchi:	InChI=1S/C12H22O2/c1-11(13)9-7-5-3-4-6-8-10-12(2)14/h3-10H2,1-2H3
InchiKey:	IALFUWZSWAKBDF-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	CC(=O)CCCCCCCCC(C)=O
Mol. weight [g/mol]:	198.30
CAS:	7029-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-207.68	kJ/mol	Joback Method
hf	-516.17	kJ/mol	Joback Method
hfus	30.03	kJ/mol	Joback Method
hvap	55.80	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.285		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
tb	581.70	K	Joback Method
tc	760.16	K	Joback Method
tf	342.90 ± 2.00	K	NIST Webbook
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.66	J/mol×K	581.70	Joback Method
cpg	476.62	J/mol×K	611.44	Joback Method
cpg	490.91	J/mol×K	641.19	Joback Method
cpg	504.54	J/mol×K	670.93	Joback Method
cpg	517.53	J/mol×K	700.67	Joback Method
cpg	529.89	J/mol×K	730.42	Joback Method
cpg	541.64	J/mol×K	760.16	Joback Method
dvisc	0.0033704	Pa×s	324.86	Joback Method
dvisc	0.0016860	Pa×s	367.67	Joback Method

dvisc	0.0009745	Pa×s	410.47	Joback Method
dvisc	0.0006247	Pa×s	453.28	Joback Method
dvisc	0.0004324	Pa×s	496.09	Joback Method
dvisc	0.0003173	Pa×s	538.89	Joback Method
dvisc	0.0002437	Pa×s	581.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7029096&Units=SI
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

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

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