

3,8-Decanedione, 2,9-dimethyl-

Inchi:	InChI=1S/C12H22O2/c1-9(2)11(13)7-5-6-8-12(14)10(3)4/h9-10H,5-8H2,1-4H3
InchiKey:	HXQGDVMNCVJPFP-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	CC(C)C(=O)CCCCC(=O)C(C)C
Mol. weight [g/mol]:	198.30
CAS:	1490-37-5

Physical Properties

Property code	Value	Unit	Source
gf	-212.56	kJ/mol	Joback Method
hf	-526.73	kJ/mol	Joback Method
hfus	22.99	kJ/mol	Joback Method
hvap	55.02	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.997		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
tb	580.82	K	Joback Method
tc	765.86	K	Joback Method
tf	294.86	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.36	J/mol×K	580.82	Joback Method
cpg	477.98	J/mol×K	611.66	Joback Method
cpg	492.86	J/mol×K	642.50	Joback Method
cpg	507.02	J/mol×K	673.34	Joback Method
cpg	520.47	J/mol×K	704.18	Joback Method
cpg	533.23	J/mol×K	735.02	Joback Method
cpg	545.33	J/mol×K	765.86	Joback Method
dvisc	0.0061035	Pa×s	294.86	Joback Method
dvisc	0.0023658	Pa×s	342.52	Joback Method

dvisc	0.0011559	Pa×s	390.18	Joback Method
dvisc	0.0006601	Pa×s	437.84	Joback Method
dvisc	0.0004208	Pa×s	485.50	Joback Method
dvisc	0.0002907	Pa×s	533.16	Joback Method
dvisc	0.0002134	Pa×s	580.82	Joback Method

Sources

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=C1490375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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