

3,5-Octanedione, 4,6-dimethyl

Inchi:	InChI=1S/C10H18O2/c1-5-7(3)10(12)8(4)9(11)6-2/h7-8H,5-6H2,1-4H3
InchiKey:	YOTJIUKJWVGJMEV-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CCC(=O)C(C)C(=O)C(C)CC
Mol. weight [g/mol]:	170.25
CAS:	37484-67-6

Physical Properties

Property code	Value	Unit	Source
gf	-229.40	kJ/mol	Joback Method
hf	-485.45	kJ/mol	Joback Method
hfus	17.81	kJ/mol	Joback Method
hvap	50.57	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.217		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1191.20		NIST Webbook
ripol	1597.00		NIST Webbook
tb	535.06	K	Joback Method
tc	724.34	K	Joback Method
tf	272.32	K	Joback Method
vc	0.596	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.42	J/molxK	535.06	Joback Method
cpg	430.08	J/molxK	692.79	Joback Method
cpg	418.43	J/molxK	661.25	Joback Method
cpg	406.15	J/molxK	629.70	Joback Method
cpg	393.24	J/molxK	598.15	Joback Method
cpg	379.67	J/molxK	566.61	Joback Method
cpg	441.12	J/molxK	724.34	Joback Method

dvisc	0.0002579	Paxs	535.06	Joback Method
dvisc	0.0003492	Paxs	491.27	Joback Method
dvisc	0.0005018	Paxs	447.48	Joback Method
dvisc	0.0007800	Paxs	403.69	Joback Method
dvisc	0.0013501	Paxs	359.90	Joback Method
dvisc	0.0027202	Paxs	316.11	Joback Method
dvisc	0.0068659	Paxs	272.32	Joback Method

Sources

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=C37484676&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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