4,6-Dimethyloctan-3,5-dione

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

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	1160.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1160.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1585.00		NIST Webbook
tb	535.06	K	Joback Method
tc	724.34	K	Joback Method
tf	272.32	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.42	J/mol×K	535.06	Joback Method
cpg	379.67	J/mol×K	566.61	Joback Method
cpg	393.24	J/mol×K	598.15	Joback Method
cpg	406.15	J/mol×K	629.70	Joback Method

cpg	418.43	J/mol×K	661.25	Joback Method
cpg	430.08	J/mol×K	692.79	Joback Method
cpg	441.12	J/mol×K	724.34	Joback Method
dvisc	0.0068659	Pa×s	272.32	Joback Method
dvisc	0.0027202	Pa×s	316.11	Joback Method
dvisc	0.0013501	Pa×s	359.90	Joback Method
dvisc	0.0007800	Pa×s	403.69	Joback Method
dvisc	0.0005018	Pa×s	447.48	Joback Method
dvisc	0.0003492	Pa×s	491.27	Joback Method
dvisc	0.0002579	Pa×s	535.06	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=R285262&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
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