Acetoin octanoate

Inchi: InChI=1S/C12H22O3/c1-4-5-6-7-8-9-12(14)15-11(3)10(2)13/h11H,4-9H2,1-3H3
InchiKey: DXTCDFXHMJNZNN-UHFFFAOYSA-N
Formula: C12H22O3
SMILES: CCCCCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 214.30

Physical Properties

Property code	Value	Unit	Source
gf	-315.12	kJ/mol	Joback Method
hf	-653.67	kJ/mol	Joback Method
hfus	27.70	kJ/mol	Joback Method
hvap	57.82	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.868		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1432.00		NIST Webbook
tb	603.68	K	Joback Method
tc	784.55	K	Joback Method
tf	332.09	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.14	J/mol×K	603.68	Joback Method
cpg	504.18	J/mol×K	633.83	Joback Method
cpg	518.53	J/mol×K	663.97	Joback Method
cpg	532.22	J/mol×K	694.12	Joback Method
cpg	545.25	J/mol×K	724.26	Joback Method

cpg	557.63	J/mol×K	754.41	Joback Method
cpg	569.37	J/mol×K	784.55	Joback Method
dvisc	0.0030790	Pa×s	332.09	Joback Method
dvisc	0.0014459	Pa×s	377.36	Joback Method
dvisc	0.0007983	Pa×s	422.62	Joback Method
dvisc	0.0004945	Pa×s	467.89	Joback Method
dvisc	0.0003333	Pa×s	513.15	Joback Method
dvisc	0.0002395	Pa×s	558.42	Joback Method
dvisc	0.0001808	Pa×s	603.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R66287&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume