

Acetoin octanoate #2

Inchi:	InChI=1S/C12H24O3/c1-4-5-6-7-8-9-12(14)15-11(3)10(2)13/h10-11,13H,4-9H2,1-3H3
InchiKey:	HPHHIFUXVYBQOZ-UHFFFAOYSA-N
Formula:	C12H24O3
SMILES:	CCCCCCCC(=O)OC(C)C(C)O
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
gf	-325.46	kJ/mol	Joback Method
hf	-698.60	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	67.36	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.659		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
tb	641.55	K	Joback Method
tc	812.55	K	Joback Method
tf	327.98	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.05	J/molxK	641.55	Joback Method
cpg	595.36	J/molxK	784.05	Joback Method
cpg	583.69	J/molxK	755.55	Joback Method
cpg	571.44	J/molxK	727.05	Joback Method
cpg	558.59	J/molxK	698.55	Joback Method
cpg	545.13	J/molxK	670.05	Joback Method
cpg	606.44	J/molxK	812.55	Joback Method
dvisc	0.0000464	Paxs	641.55	Joback Method

dvisc	0.0000764	Paxs	589.29	Joback Method
dvisc	0.0001385	Paxs	537.03	Joback Method
dvisc	0.0002856	Paxs	484.76	Joback Method
dvisc	0.0007012	Paxs	432.50	Joback Method
dvisc	0.0022042	Paxs	380.24	Joback Method
dvisc	0.0099801	Paxs	327.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R66291&Units=SI

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

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