(Z)-3-(Hydroxymethyl)-7-methylocta-2,6-dien-1-yl acetate

Inchi: InChI=1S/C12H20O3/c1-10(2)5-4-6-12(9-13)7-8-15-11(3)14/h5,7,13H,4,6,8-9H2,1-3H3/b
InchiKey: YSJLKCJDEAYOME-GHXNOFRVSA-N
Formula: C12H20O3
SMILES: CC(=O)OCC=C(CO)CCC=C(C)C
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-177.24	kJ/mol	Joback Method
hf	-473.18	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.215		Crippen Method
mcvol	184.650	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
ripol	1764.00		NIST Webbook
tb	650.51	K	Joback Method
tc	831.83	K	Joback Method
tf	319.90	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.58	J/mol×K	650.51	Joback Method
cpg	499.45	J/mol×K	680.73	Joback Method
cpg	511.70	J/mol×K	710.95	Joback Method
cpg	523.35	J/mol×K	741.17	Joback Method
cpg	534.43	J/mol×K	771.39	Joback Method
cpg	544.98	J/mol×K	801.61	Joback Method
cpg	555.01	J/mol×K	831.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519154&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume