(5E,8E,11E)-tetradecatrien-2-one

Inchi: InChI=1S/C14H22O/c1-3-4-5-6-7-8-9-10-11-12-13-14(2)15/h4-5,7-8,10-11H,3,6,9,12-13H
InchiKey: IVCSDEBPVQZWOF-JSIPCRQOSA-N
Formula: C14H22O
SMILES: CCC=CCC=CCC=CCCC(C)=O
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	178.74	kJ/mol	Joback Method
hf	-93.21	kJ/mol	Joback Method
hfus	34.22	kJ/mol	Joback Method
hvap	53.38	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.214		Crippen Method
mcvol	196.790	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
ripol	2033.00		NIST Webbook
ripol	2033.00		NIST Webbook
tb	586.07	K	Joback Method
tc	774.12	K	Joback Method
tf	282.23	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.20	J/mol×K	586.07	Joback Method
cpg	496.22	J/mol×K	617.41	Joback Method
cpg	511.39	J/mol×K	648.75	Joback Method
cpg	525.76	J/mol×K	680.10	Joback Method
cpg	539.38	J/mol×K	711.44	Joback Method
cpg	552.30	J/mol×K	742.78	Joback Method
cpg	564.58	J/mol×K	774.12	Joback Method
dvisc	0.0032895	Pa×s	282.23	Joback Method

dvisc	0.0012442	Pa×s	332.87	Joback Method
dvisc	0.0006084	Pa×s	383.51	Joback Method
dvisc	0.0003515	Pa×s	434.15	Joback Method
dvisc	0.0002278	Pa×s	484.79	Joback Method
dvisc	0.0001602	Pa×s	535.43	Joback Method
dvisc	0.0001198	Pa×s	586.07	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=R297780&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume