

(5Z,8Z,11Z)-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-YSTUJMKBSA-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	2014.00		NIST Webbook
ripol	2014.00		NIST Webbook
tb	586.07	K	Joback Method
tc	774.12	K	Joback Method
tf	282.23	K	Joback Method
vc	0.765	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0012442	Paxs	332.87	Joback Method
dvisc	0.0006084	Paxs	383.51	Joback Method
dvisc	0.0003515	Paxs	434.15	Joback Method
dvisc	0.0002278	Paxs	484.79	Joback Method
dvisc	0.0001602	Paxs	535.43	Joback Method
dvisc	0.0001198	Paxs	586.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R297859&Units=SI
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

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

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