5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-

Other names: 5,9,13-Pentadecatriene-2-one, 6,10,14-trimethyl-
Pentadeca-5,9,13-triene-2-one, 6,10,14-trimethyl-
6,10,14-Trimethyl-5,9,13-pentadecatrien-2-one
6,10,14-trimethylpentadeca-5,9,13-trien-2-one
Inchi: InChI=1S/C18H30O/c1-15(2)9-6-10-16(3)11-7-12-17(4)13-8-14-18(5)19/h9,11,13H,6-8,1
InchiKey: LTUMRKDLVGQMJU-UHFFFAOYSA-N
Formula: C18H30O
SMILES: CC(=O)CCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 262.43
CAS: 762-29-8

Physical Properties

Property code	Value	Unit	Source
gf	186.77	kJ/mol	Joback Method
hf	-205.14	kJ/mol	Joback Method
hfus	40.65	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.775		Crippen Method
mcvol	253.150	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	1921.00		NIST Webbook
tb	677.23	K	Joback Method
tc	866.12	K	Joback Method
tf	285.43	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.45	J/mol×K	677.23	Joback Method
cpg	710.76	J/mol×K	708.71	Joback Method
cpg	728.14	J/mol×K	740.19	Joback Method
cpg	744.65	J/mol×K	771.68	Joback Method

cpg	760.37	J/mol×K	803.16	Joback Method
cpg	775.34	J/mol×K	834.64	Joback Method
cpg	789.64	J/mol×K	866.12	Joback Method

Sources

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=C762298&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume