2,4,6,9-Tetramethyldec-8-en-3,5-dion (A)

Inchi: InChI=1S/C14H24O2/c1-9(2)7-8-11(5)14(16)12(6)13(15)10(3)4/h7,10-12H,8H2,1-6H3
InchiKey: VNEFXHWAHYWLHU-UHFFFAOYSA-N
Formula: C14H24O2
SMILES: CC(C)=CCC(C)C(=O)C(C)C(=O)C(C)C
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	-126.49	kJ/mol	Joback Method
hf	-465.86	kJ/mol	Joback Method
hfus	23.54	kJ/mol	Joback Method
hvap	59.12	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.409		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1464.00		NIST Webbook
rinpol	1464.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1882.00		NIST Webbook
tb	630.18	K	Joback Method
tc	824.55	K	Joback Method
tf	283.36	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.13	J/mol×K	630.18	Joback Method
cpg	561.92	J/mol×K	662.57	Joback Method
cpg	577.81	J/mol×K	694.97	Joback Method
cpg	592.84	J/mol×K	727.36	Joback Method
cpg	607.05	J/mol×K	759.76	Joback Method
cpg	620.47	J/mol×K	792.15	Joback Method

cpg	633.14	J/mol×K	824.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R285277&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume