1,2,4-Cyclopentanetrione, 3,3-bis(3-methyl-2-butenyl)-5-(2-methyl-1-oxoprop

Other names: 1,2,4-Cyclopentanetrione, 5-isobutyryl-3,3-bis(3-methyl-2-butenyl)-
Cohulupone
Cohulupon

Inchi: InChI=1S/C19H26O4/c1-11(2)7-9-19(10-8-12(3)4)17(22)14(15(20)13(5)6)16(21)18(19)23

InchiKey: HMEGPOIWNGKXBR-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: CC(C)=CCC1(CC=C(C)C)C(=O)C(=O)C(C(=O)C(C)C)C1=O

Mol. weight [g/mol]: 318.41

CAS: 1891-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-223.34	kJ/mol	Joback Method
hf	-696.21	kJ/mol	Joback Method
hfus	28.06	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.248		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	909.94	K	Joback Method
tc	1147.74	K	Joback Method
tf	535.96	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.44	J/mol×K	909.94	Joback Method
cpg	898.16	J/mol×K	949.57	Joback Method
cpg	917.06	J/mol×K	989.21	Joback Method
cpg	935.25	J/mol×K	1028.84	Joback Method

cpg	952.84	J/mol×K	1068.47	Joback Method
cpg	969.92	J/mol×K	1108.10	Joback Method
cpg	986.60	J/mol×K	1147.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1891345&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

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