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

Other names:	1,2,4-Cyclopentanetrione, 5-isovaleryl-3,3-bis(3-methyl-2-butenyl)- Hulupone 1,3-Cyclopentanedione, 4-hydroxy-2,2-bis(3-methyl-2-butenyl)-5-(3-methyl-1-oxobutyl)-
Inchi:	InChI=1S/C20H28O4/c1-12(2)7-9-20(10-8-13(3)4)18(23)16(17(22)19(20)24)15(21)11-14
InchiKey:	SGJIYESRGDTFSD-UHFFFAOYSA-N
Formula:	C20H28O4
SMILES:	CC(C)=CCC1(CC=C(C)C)C(=O)C(=O)C(C(=O)CC(C)C)C1=O
Mol. weight [g/mol]:	332.43
CAS:	468-62-2

Physical Properties

Property code	Value	Unit	Source
gf	-214.92	kJ/mol	Joback Method
hf	-716.85	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	78.09	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.638		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2124.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	2103.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	932.82	K	Joback Method
tc	1168.49	K	Joback Method
tf	547.23	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.96	J/mol×K	932.82	Joback Method

cpg	959.96	J/mol×K	972.10	Joback Method
cpg	979.16	J/mol×K	1011.38	Joback Method
cpg	997.66	J/mol×K	1050.66	Joback Method
cpg	1015.57	J/mol×K	1089.94	Joback Method
cpg	1032.99	J/mol×K	1129.21	Joback Method
cpg	1050.02	J/mol×K	1168.49	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=C468622&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
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

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