Curdione

Other names:	6,10-Dimethyl-3-(1-methylethyl)-6-cyclodecene-1,4-dione, (3S-(3R*,6E,10R*))-3-Isopropyl-6,10-dimethyl-6-cyclodecene-1,4-dione, (3S-(3R*,6E,10R*))-3S,6E,10S)-6,10-Dimethyl-3-propan-2-ylcyclodec-6-ene-1,4-dione Germacr-1(10)-ene-5,8-dione
Inchi:	InChI=1S/C15H24O2/c1-10(2)13-9-14(16)12(4)7-5-6-11(3)8-15(13)17/h6,10,12-13H,5,7-
InchiKey:	KDPFMRXIVDLQKX-WDZFZDKYSA-N
Formula:	C15H24O2
SMILES:	CC1=CCCC(C)C(=O)CC(C(C)C)C(=O)C1
Mol. weight [g/mol]:	236.35
CAS:	13657-68-6

Physical Properties

Property code	Value	Unit	Source
gf	-183.53	kJ/mol	Joback Method
hf	-577.96	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.553		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1725.20		NIST Webbook
tb	713.90	K	Joback Method
tc	956.91	K	Joback Method
tf	382.59	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.90	J/mol×K	713.90	Joback Method
cpg	654.71	J/mol×K	754.40	Joback Method
cpg	676.68	J/mol×K	794.90	Joback Method
cpg	696.72	J/mol×K	835.40	Joback Method
cpg	714.74	J/mol×K	875.90	Joback Method
cpg	730.66	J/mol×K	916.41	Joback Method
cpg	744.39	J/mol×K	956.91	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=C13657686&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