

3,5,7,10-Tetramethylundec-9-ene-4,6-dione

Other names:	3,5,7,10-tetramethylundec-9-ene-4,6-dione
Inchi:	InChI=1S/C15H26O2/c1-7-11(4)14(16)13(6)15(17)12(5)9-8-10(2)3/h8,11-13H,7,9H2,1-6H1
InchiKey:	BZBFBQMTXDLSPW-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	CCC(C)C(=O)C(C)C(=O)C(C)CC=C(C)C
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
hf	-539.32	kJ/mol	Cheméo Relay (1.0)
hfus	26.13	kJ/mol	Joback Method
hvap	66.34	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-3.47		Cheméo Relay (1.0)
logp	3.799		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
tb	533.96	K	Cheméo Relay (1.0)
tc	716.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.33	J/mol×K	653.06	Joback Method
cpg	615.53	J/mol×K	685.10	Joback Method
cpg	631.82	J/mol×K	717.14	Joback Method
cpg	647.23	J/mol×K	749.18	Joback Method
cpg	661.80	J/mol×K	781.22	Joback Method
cpg	675.58	J/mol×K	813.26	Joback Method
cpg	688.59	J/mol×K	845.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13851086&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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