3,5,7,10-Tetramethylundec-9-en-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,7,9H2,1-6
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
CAS: 13851-08-6

Physical Properties

Property code	Value	Unit	Source
gf	-118.07	kJ/mol	Joback Method
hf	-486.50	kJ/mol	Joback Method
hfus	26.13	kJ/mol	Joback Method
hvap	61.35	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.799		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	1553.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1582.70		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1582.70		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1950.00		NIST Webbook
tb	653.06	K	Joback Method
tc	845.30	K	Joback Method
tf	294.63	K	Joback Method
vc	0.851	m3/kmol	Joback Method

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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13851086&Units=SI

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