5,7,10-Trimethylundec-9-en-4,6-dione

Other names: 9-Undecen-4,6-dione, 5,7,10-trimethyl
5,7,10-trimethylundec-9-ene-4,6-dione
Inchi: InChI=1S/C14H24O2/c1-6-7-13(15)12(5)14(16)11(4)9-8-10(2)3/h8,11-12H,6-7,9H2,1-5H
InchiKey: CFGSDQZJQUFHTO-UHFFFAOYSA-N
Formula: C14H24O2
SMILES: CCCC(=O)C(C)C(=O)C(C)CC=C(C)C
Mol. weight [g/mol]: 224.34
CAS: 94201-70-4

Physical Properties

Property code	Value	Unit	Source
gf	-124.05	kJ/mol	Joback Method
hf	-460.58	kJ/mol	Joback Method
hfus	27.06	kJ/mol	Joback Method
hvap	59.51	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.553		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	1493.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1493.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1869.00		NIST Webbook
tb	630.62	K	Joback Method
tc	821.58	K	Joback Method
tf	298.36	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.71	J/mol×K	630.62	Joback Method
cpg	561.16	J/mol×K	662.45	Joback Method

cpg	576.76	J/mol×K	694.27	Joback Method
cpg	591.53	J/mol×K	726.10	Joback Method
cpg	605.52	J/mol×K	757.93	Joback Method
cpg	618.75	J/mol×K	789.76	Joback Method
cpg	631.27	J/mol×K	821.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94201704&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume