

2,5,7-trimethyl-2-decene-6,8-dione

Other names:	4,6,9-Trimethyldec-8-en-3,5-dione
Inchi:	InChI=1S/C13H22O2/c1-6-12(14)11(5)13(15)10(4)8-7-9(2)3/h7,10-11H,6,8H2,1-5H3
InchiKey:	IJGCQHHZHMDOD-UHFFFAOYSA-N
Formula:	C13H22O2
SMILES:	CCC(=O)C(C)C(=O)C(C)CC=C(C)C
Mol. weight [g/mol]:	210.31
CAS:	13851-06-4

Physical Properties

Property code	Value	Unit	Source
gf	-132.47	kJ/mol	Joback Method
hf	-439.94	kJ/mol	Joback Method
hfus	24.47	kJ/mol	Joback Method
hvap	57.29	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.163		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1449.10		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1449.10		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1865.00		NIST Webbook
tb	607.74	K	Joback Method
tc	800.90	K	Joback Method
tf	287.09	K	Joback Method
vc	0.745	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.92	J/mol×K	607.74	Joback Method
cpg	508.89	J/mol×K	639.93	Joback Method
cpg	524.01	J/mol×K	672.13	Joback Method
cpg	538.33	J/mol×K	704.32	Joback Method
cpg	551.89	J/mol×K	736.51	Joback Method
cpg	564.70	J/mol×K	768.71	Joback Method
cpg	576.81	J/mol×K	800.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13851064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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