Trimenal

Inchi: InChI=1S/C13H22O/c1-11(2)6-5-7-12(3)8-9-13(4)10-14/h8,10,13H,1,5-7,9H2,2-4H3/b12-
InchiKey: MINJGYRWHNAENM-WQLSENKSSA-N
Formula: C13H22O
SMILES: C=C(C)CCCC(C)=CCC(C)C=O
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	107.58	kJ/mol	Joback Method
hf	-179.44	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hvap	50.31	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.904		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
tb	545.66	K	Joback Method
tc	729.69	K	Joback Method
tf	228.51	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.94	J/mol×K	545.66	Joback Method
cpg	464.18	J/mol×K	576.33	Joback Method
cpg	479.61	J/mol×K	607.00	Joback Method
cpg	494.27	J/mol×K	637.68	Joback Method
cpg	508.19	J/mol×K	668.35	Joback Method
cpg	521.41	J/mol×K	699.02	Joback Method
cpg	533.98	J/mol×K	729.69	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=R277706&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