Henicosane-2,4-dione

Inchi: InChI=1S/C21H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21(23)19-20(2)22/h3
InchiKey: ZBRRLVWJAPULGW-UHFFFAOYSA-N
Formula: C21H40O2
SMILES: CCCCCCCCCCCCCCCCCCC(=O)CC(C)=O
Mol. weight [g/mol]: 324.54
CAS: 6136-88-5

Physical Properties

Property code	Value	Unit	Source
gf	-131.90	kJ/mol	Joback Method
hf	-701.93	kJ/mol	Joback Method
hfus	53.34	kJ/mol	Joback Method
hvap	75.83	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.796		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1035.23	kPa	Joback Method
rinpol	2412.70		NIST Webbook
tb	787.62	K	Joback Method
tc	968.12	K	Joback Method
tf	426.29	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.81	J/mol×K	787.62	Joback Method
cpg	984.87	J/mol×K	817.70	Joback Method
cpg	1002.96	J/mol×K	847.79	Joback Method
cpg	1020.10	J/mol×K	877.87	Joback Method
cpg	1036.34	J/mol×K	907.95	Joback Method
cpg	1051.71	J/mol×K	938.04	Joback Method
cpg	1066.24	J/mol×K	968.12	Joback Method
dvisc	0.0016307	Pa×s	426.29	Joback Method

dvisc	0.0007274	Pa×s	486.51	Joback Method
dvisc	0.0003876	Pa×s	546.73	Joback Method
dvisc	0.0002340	Pa×s	606.96	Joback Method
dvisc	0.0001548	Pa×s	667.18	Joback Method
dvisc	0.0001096	Pa×s	727.40	Joback Method
dvisc	0.0000818	Pa×s	787.62	Joback Method

Sources

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=C6136885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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