

Hentriacontan-2,4-dione

Inchi:	InChI=1S/C31H60O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	ABMKZUGNXZKOAK-UHFFFAOYSA-N
Formula:	C31H60O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)CC(C)=O
Mol. weight [g/mol]:	464.81
CAS:	112468-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-47.70	kJ/mol	Joback Method
hf	-908.33	kJ/mol	Joback Method
hfus	79.24	kJ/mol	Joback Method
hvap	98.09	kJ/mol	Joback Method
log10ws	-11.36		Crippen Method
logp	10.697		Crippen Method
mvol	450.790	ml/mol	McGowan Method
pc	604.28	kPa	Joback Method
rinpol	3441.70		NIST Webbook
rinpol	3441.70		NIST Webbook
tb	1016.42	K	Joback Method
tc	1271.51	K	Joback Method
tf	538.99	K	Joback Method
vc	1.784	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1607.38	J/molxK	1016.42	Joback Method
cpg	1720.40	J/molxK	1228.99	Joback Method
cpg	1701.12	J/molxK	1186.48	Joback Method
cpg	1680.34	J/molxK	1143.96	Joback Method
cpg	1657.89	J/molxK	1101.45	Joback Method
cpg	1633.62	J/molxK	1058.93	Joback Method
cpg	1738.33	J/molxK	1271.51	Joback Method

dvisc	0.0000183	Paxs	1016.42	Joback Method
dvisc	0.0000249	Paxs	936.85	Joback Method
dvisc	0.0000361	Paxs	857.28	Joback Method
dvisc	0.0000562	Paxs	777.70	Joback Method
dvisc	0.0000970	Paxs	698.13	Joback Method
dvisc	0.0001927	Paxs	618.56	Joback Method
dvisc	0.0004684	Paxs	538.99	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=C112468367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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

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