

Henicosane-6,8-dione

Inchi:	InChI=1S/C21H40O2/c1-3-5-7-8-9-10-11-12-13-14-16-18-21(23)19-20(22)17-15-6-4-2/h3
InchiKey:	MRBZNGRWKALXEA-UHFFFAOYSA-N
Formula:	C21H40O2
SMILES:	CCCCCCCCCCCCC(=O)CC(=O)CCCCC
Mol. weight [g/mol]:	324.54
CAS:	289681-92-1

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	2379.50		NIST Webbook
rinpol	2379.50		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/molxK	787.62	Joback Method
cpg	984.87	J/molxK	817.70	Joback Method
cpg	1002.96	J/molxK	847.79	Joback Method
cpg	1020.10	J/molxK	877.87	Joback Method
cpg	1036.34	J/molxK	907.95	Joback Method
cpg	1051.71	J/molxK	938.04	Joback Method
cpg	1066.24	J/molxK	968.12	Joback Method

dvisc	0.0016307	Paxs	426.29	Joback Method
dvisc	0.0007274	Paxs	486.51	Joback Method
dvisc	0.0003876	Paxs	546.73	Joback Method
dvisc	0.0002340	Paxs	606.96	Joback Method
dvisc	0.0001548	Paxs	667.18	Joback Method
dvisc	0.0001096	Paxs	727.40	Joback Method
dvisc	0.0000818	Paxs	787.62	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=C289681921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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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