

Triacontane-7,9-dione

Inchi: InChI=1S/C30H58O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-27-30(24-26-28)
InchiKey: KUWSHTWTAAEVLN-UHFFFAOYSA-N
Formula: C30H58O2
SMILES: CCCCCCCCCCCCCCCCCCCCCC(=O)CC(=O)CCCCC
Mol. weight [g/mol]: 450.78

Physical Properties

Property code	Value	Unit	Source
gf	-56.12	kJ/mol	Joback Method
hf	-887.69	kJ/mol	Joback Method
hfus	76.65	kJ/mol	Joback Method
hvap	95.87	kJ/mol	Joback Method
log10ws	-10.94		Crippen Method
logp	10.307		Crippen Method
mvol	436.700	ml/mol	McGowan Method
pc	633.84	kPa	Joback Method
rinpol	3307.20		NIST Webbook
rinpol	3307.20		NIST Webbook
tb	993.54	K	Joback Method
tc	1235.72	K	Joback Method
tf	527.72	K	Joback Method
vc	1.728	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1540.94	J/molxK	993.54	Joback Method
cpg	1566.11	J/molxK	1033.90	Joback Method
cpg	1589.48	J/molxK	1074.27	Joback Method
cpg	1611.16	J/molxK	1114.63	Joback Method
cpg	1631.30	J/molxK	1155.00	Joback Method
cpg	1650.02	J/molxK	1195.36	Joback Method
cpg	1667.46	J/molxK	1235.72	Joback Method
dvisc	0.0005374	Paxs	527.72	Joback Method

dvisc	0.0002225	Paxs	605.36	Joback Method
dvisc	0.0001126	Paxs	682.99	Joback Method
dvisc	0.0000655	Paxs	760.63	Joback Method
dvisc	0.0000421	Paxs	838.27	Joback Method
dvisc	0.0000292	Paxs	915.90	Joback Method
dvisc	0.0000214	Paxs	993.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414340&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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