Docosanal

Inchi: InChI=1S/C22H44O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23/h22
InchiKey: ULCXRAFXRZTNRO-UHFFFAOYSA-N
Formula: C22H44O
SMILES: CCCCCCCCCCCCCCCCCCCCCC=O
Mol. weight [g/mol]: 324.58
CAS: 57402-36-5

Physical Properties

Property code	Value	Unit	Source
gf	34.84	kJ/mol	Joback Method
hf	-582.99	kJ/mol	Joback Method
hfus	55.02	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	8.007		Crippen Method
mcvol	322.410	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	2426.00		NIST Webbook
rinpol	2434.00		NIST Webbook
tb	751.42	K	Joback Method
tc	923.06	K	Joback Method
tf	379.70	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	995.54	J/mol×K	751.42	Joback Method
cpg	1016.13	J/mol×K	780.03	Joback Method
cpg	1035.77	J/mol×K	808.63	Joback Method
cpg	1054.48	J/mol×K	837.24	Joback Method
cpg	1072.31	J/mol×K	865.85	Joback Method
cpg	1089.28	J/mol×K	894.46	Joback Method
cpg	1105.44	J/mol×K	923.06	Joback Method

dvisc	0.0023559	Pa×s	379.70	Joback Method
dvisc	0.0009101	Pa×s	441.65	Joback Method
dvisc	0.0004442	Pa×s	503.61	Joback Method
dvisc	0.0002538	Pa×s	565.56	Joback Method
dvisc	0.0001619	Pa×s	627.51	Joback Method
dvisc	0.0001120	Pa×s	689.47	Joback Method
dvisc	0.0000823	Pa×s	751.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57402365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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