9,12,15-Octadecatrienal

Other names: Octadeca-9,12,15-trienal
Inchi: InChI=1S/C18H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h3-4,6-7,9-10,18
InchiKey: TUCMDDWTBVMRTP-IUQGRGSQSA-N
Formula: C18H30O
SMILES: CCC=CCC=CCC=CCCCCCCCC=O
Mol. weight [g/mol]: 262.43
CAS: 26537-71-3

Physical Properties

Property code	Value	Unit	Source
gf	241.82	kJ/mol	Joback Method
hf	-148.77	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	62.26	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.775		Crippen Method
mcvol	253.150	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	2109.00		NIST Webbook
rinpol	2045.00		NIST Webbook
rinpol	2061.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	672.38	K	Joback Method
tc	851.25	K	Joback Method
tf	319.38	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.79	J/mol×K	672.38	Joback Method
cpg	710.24	J/mol×K	702.19	Joback Method
cpg	726.84	J/mol×K	732.00	Joback Method
cpg	742.65	J/mol×K	761.81	Joback Method

cpg	757.72	J/mol×K	791.62	Joback Method
cpg	772.11	J/mol×K	821.43	Joback Method
cpg	785.87	J/mol×K	851.25	Joback Method
dvisc	0.0028878	Pa×s	319.38	Joback Method
dvisc	0.0010250	Pa×s	378.21	Joback Method
dvisc	0.0004808	Pa×s	437.05	Joback Method
dvisc	0.0002699	Pa×s	495.88	Joback Method
dvisc	0.0001713	Pa×s	554.71	Joback Method
dvisc	0.0001186	Pa×s	613.55	Joback Method
dvisc	0.0000876	Pa×s	672.38	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26537713&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

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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