

(Z,Z,Z)-8,11,14-Heptadecatrienal

Other names:	(8Z,11Z,14Z)-Heptadecatrienal
Inchi:	InChI=1S/C17H28O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h3-4,6-7,9-10,17H,2
InchiKey:	NIPNNUONNZABRE-PDBXOOCHSA-N
Formula:	C17H28O
SMILES:	CCC=CCC=CCC=CCCCCCC=O
Mol. weight [g/mol]:	248.40

Physical Properties

Property code	Value	Unit	Source
gf	233.40	kJ/mol	Joback Method
hf	-128.13	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.385		Crippen Method
mvol	239.060	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinpol	1852.00		NIST Webbook
rinpol	1874.00		NIST Webbook
tb	649.50	K	Joback Method
tc	829.17	K	Joback Method
tf	308.11	K	Joback Method
vc	0.945	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.68	J/mol×K	649.50	Joback Method
cpg	715.11	J/mol×K	799.22	Joback Method
cpg	701.10	J/mol×K	769.28	Joback Method
cpg	686.40	J/mol×K	739.33	Joback Method
cpg	670.97	J/mol×K	709.39	Joback Method
cpg	654.74	J/mol×K	679.44	Joback Method
cpg	728.49	J/mol×K	829.17	Joback Method

dvisc	0.0000978	Paxs	649.50	Joback Method
dvisc	0.0001321	Paxs	592.60	Joback Method
dvisc	0.0001901	Paxs	535.70	Joback Method
dvisc	0.0002984	Paxs	478.81	Joback Method
dvisc	0.0005290	Paxs	421.91	Joback Method
dvisc	0.0011210	Paxs	365.01	Joback Method
dvisc	0.0031347	Paxs	308.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R263524&Units=SI

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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