

(Z,E)-6,8-heneicosadien-11-one

Inchi:	InChI=1S/C21H38O/c1-3-5-7-9-11-13-15-17-19-21(22)20-18-16-14-12-10-8-6-4-2/h11,13
InchiKey:	OOYMTGLPPRCUKK-WREYUNAZSA-N
Formula:	C21H38O
SMILES:	CCCCC=CC=CCC(=O)CCCCCCCCC
Mol. weight [g/mol]:	306.53

Physical Properties

Property code	Value	Unit	Source
gf	157.46	kJ/mol	Joback Method
hf	-354.91	kJ/mol	Joback Method
hfus	52.15	kJ/mol	Joback Method
hvap	69.00	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.169		Crippen Method
mcvol	299.720	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinpol	2300.00		NIST Webbook
tb	742.07	K	Joback Method
tc	919.79	K	Joback Method
tf	366.20	K	Joback Method
vc	1.177	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.59	J/mol×K	742.07	Joback Method
cpg	908.84	J/mol×K	771.69	Joback Method
cpg	927.18	J/mol×K	801.31	Joback Method
cpg	944.67	J/mol×K	830.93	Joback Method
cpg	961.35	J/mol×K	860.55	Joback Method
cpg	977.28	J/mol×K	890.17	Joback Method
cpg	992.50	J/mol×K	919.79	Joback Method
dvisc	0.0019719	Paxs	366.20	Joback Method
dvisc	0.0007314	Paxs	428.85	Joback Method

dvisc	0.0003493	Paxs	491.49	Joback Method
dvisc	0.0001971	Paxs	554.13	Joback Method
dvisc	0.0001250	Paxs	616.78	Joback Method
dvisc	0.0000862	Paxs	679.43	Joback Method
dvisc	0.0000633	Paxs	742.07	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=R413888&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
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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