8E,15E,22E-heptatriaconta-trien-2-one

Other names: Heptatriaconta-8E,15E,22E-trien-2-one
Inchi: InChI=1S/C37H68O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey: BVZVGJNVBQWQNU-OVNHWCOASA-N
Formula: C37H68O
SMILES: CCCCCCCCCCCCCCC=CCCCCCC=CCCCCCC=CCCCCCC(C)=O
Mol. weight [g/mol]: 528.94

Physical Properties

Property code	Value	Unit	Source
gf	372.40	kJ/mol	Joback Method
hf	-567.93	kJ/mol	Joback Method
hfus	93.79	kJ/mol	Joback Method
hvap	104.58	kJ/mol	Joback Method
log10ws	-14.15		Crippen Method
logp	13.187		Crippen Method
mcvol	520.860	ml/mol	McGowan Method
pc	482.82	kPa	Joback Method
rinpol	3883.00		NIST Webbook
rinpol	3883.00		NIST Webbook
rinpol	3883.00		NIST Webbook
tb	1112.31	K	Joback Method
tc	1424.96	K	Joback Method
tf	541.44	K	Joback Method
vc	2.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1908.72	J/mol×K	1112.31	Joback Method
cpg	2076.37	J/mol×K	1372.85	Joback Method
cpg	2043.73	J/mol×K	1320.74	Joback Method
cpg	2011.12	J/mol×K	1268.63	Joback Method
cpg	1978.07	J/mol×K	1216.53	Joback Method
cpg	1944.09	J/mol×K	1164.42	Joback Method

cpg	2109.53	J/mol×K	1424.96	Joback Method
dvisc	0.0000052	Pa×s	1112.31	Joback Method
dvisc	0.0000072	Pa×s	1017.16	Joback Method
dvisc	0.0000108	Pa×s	922.02	Joback Method
dvisc	0.0000177	Pa×s	826.88	Joback Method
dvisc	0.0000330	Pa×s	731.73	Joback Method
dvisc	0.0000743	Pa×s	636.59	Joback Method
dvisc	0.0002222	Pa×s	541.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407353&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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