

8E,15E,22E,29E-heptatriaconta-tetraen-2-one

Other names:	Heptatriaconta-8E,15E,22E,29E-tetraen-2-one
Inchi:	InChI=1S/C37H66O/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:	DPRXWDBEWOTBA-UGGLBSCLSA-N
Formula:	C37H66O
SMILES:	CCCCCCCC=CCCCCCC=CCCCCCC=CCCCCCC=CCCCCCC(C)=O
Mol. weight [g/mol]:	526.92

Physical Properties

Property code	Value	Unit	Source
gf	452.62	kJ/mol	Joback Method
hf	-450.71	kJ/mol	Joback Method
hfus	93.99	kJ/mol	Joback Method
hvap	104.53	kJ/mol	Joback Method
log10ws	-14.01		Crippen Method
logp	12.963		Crippen Method
mvol	516.560	ml/mol	McGowan Method
pc	494.05	kPa	Joback Method
rinpol	3866.00		NIST Webbook
rinpol	3866.00		NIST Webbook
tb	1116.47	K	Joback Method
tc	1422.23	K	Joback Method
tf	536.36	K	Joback Method
vc	2.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1881.26	J/molxK	1116.47	Joback Method
cpg	2053.27	J/molxK	1371.27	Joback Method
cpg	2018.70	J/molxK	1320.31	Joback Method
cpg	1984.70	J/molxK	1269.35	Joback Method
cpg	1950.78	J/molxK	1218.39	Joback Method
cpg	1916.46	J/molxK	1167.43	Joback Method
cpg	2088.89	J/molxK	1422.23	Joback Method

dvisc	0.0000046	Paxs	1116.47	Joback Method
dvisc	0.0000064	Paxs	1019.79	Joback Method
dvisc	0.0000096	Paxs	923.10	Joback Method
dvisc	0.0000157	Paxs	826.41	Joback Method
dvisc	0.0000296	Paxs	729.73	Joback Method
dvisc	0.0000677	Paxs	633.05	Joback Method
dvisc	0.0002082	Paxs	536.36	Joback Method

Sources

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=R407348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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