«beta» Carotene

Other names:

(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-1,18-bis(2,6,6-trimethyl-1-cycl
(all-E)-1,1'-(3,7,12,16-Tetramethyl-1,3,5,7,9,11,13,15,17-octadecanonaene-1,18-diyl)bis(2
.beta.-carotene

1,1'-(3,7,12,16-Tetramethyl-1,3,5,7,9,11,13,15,17-octadecanonaene-1,18-diyl)bis(2,6,6-tr
BetaVit
(all E)-
Betacarotene
C.I. 75130
C.I. Food Orange 5
Carotaben
Carotene, «beta»
Cyclohexene,
1,1'-(3,7,12,16-tetramethyl-1,3,5,7,9,11,13,15,17-octadecanonaene-1,18-diyl)bis[2,6,6-trim
Food Orange 5
(all-E)-
KPMK
Karotin
Lucaratin
NSC 62794
Natural yellow 26
Provatene
Provitamin A
Serlabo
Solatene
Zlut prirodni 26
all-E-«beta»-Carotene
all-trans-«beta»-Carotene
beta,beta-Carotene
trans-«beta»-Carotene
«beta»,«beta»-Carotene
«beta»-Carotene, all-trans-

Inchi: InChI=1S/C40H56/c1-31(19-13-21-33(3)25-27-37-35(5)23-15-29-39(37,7)8)17-11-12-18-

InchiKey: OENHQHLEOONYIE-JLTXGRSLSA-N

Formula: C40H56

SMILES: CC(C=CC=C(C)C=CC1=C(C)CCCC1(C)C)=CC=CC=C(C)C=CC=C(C)C=CC1=C(C)CCC

Mol. weight [g/mol]: 536.87

CAS: 7235-40-7

Physical Properties

Property code	Value	Unit	Source

gf	1033.02	kJ/mol	Joback Method
hf	355.69	kJ/mol	Joback Method
hfus	67.90	kJ/mol	Joback Method
hvap	106.36	kJ/mol	Joback Method
ie	6.50	eV	NIST Webbook
log10ws	-14.26		Crippen Method
logp	12.606		Crippen Method
mcvol	505.440	ml/mol	McGowan Method
pc	607.26	kPa	Joback Method
tb	1209.38	K	Joback Method
tc	1480.86	K	Joback Method
tf	553.16	K	Joback Method
vc	1.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1963.97	J/mol×K	1209.38	Joback Method
cpg	2029.84	J/mol×K	1254.63	Joback Method
cpg	2101.86	J/mol×K	1299.87	Joback Method
cpg	2180.85	J/mol×K	1345.12	Joback Method
cpg	2267.57	J/mol×K	1390.37	Joback Method
cpg	2362.84	J/mol×K	1435.61	Joback Method
cpg	2467.42	J/mol×K	1480.86	Joback Method
hfust	56.00	kJ/mol	456.00	NIST Webbook

Sources

Solubility of -Carotene in Binary Solvents Formed by Some Hydrocarbons with Dibutyl Ether and 1,2-Dimethoxyethane:	https://www.doi.org/10.1021/je030165y
Solubility of b-carotene in ethanol, and tribein-modified CO2:	https://www.doi.org/10.1016/j.jct.2011.07.013
Solubility of a-Carotene in Binary Solvents Formed by Some Hydrocarbons with 2,5,8-Trioxanonane, 2-Propanone, and Cyclohexanone:	https://www.doi.org/10.1021/je060376d
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7235407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
High-Pressure Vapor-Liquid Equilibrium Data for Systems Involving Carbon Dioxide + Organic Solvent + a-Carotene:	https://www.doi.org/10.1021/je700125v
Solubility of beta -Carotene and Glyceryl Trioleate Mixture in Supercritical CO2:	https://www.doi.org/10.1021/je400553y
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Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Solubility of a-Carotene in Binary Solvents Formed by Some Hydrocarbons with tert-Butyl Methyl Ether and Tert-Amyl Methyl Ether: https://www.doi.org/10.1021/je0495583

Solubilities and Adsorption Equilibria of beta-Carotene in Supercritical and Near-Critical Fluids: https://www.doi.org/10.1021/je100229f

Densities of a-Carotene-Supercritical Carbon Dioxide Mixtures: https://www.doi.org/10.1021/je700373r

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume