(S,Z)-Heptadeca-1,9-dien-4,6-diyn-3-ol

Other names:	(+)-Falcarinol
	Falcarinol
	1,9-Heptadecadiene-4,6-diyn-3-ol, (3S,9Z)-
	Heptadeca-1,9-dien-4,6-diyn-3-ol
Inchi:	InChI=1S/C17H24O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17(18)4-2/h4,10-11,17-18H,2-
InchiKey:	UGJAEDFOKNAMQD-QXPKXGMISA-N
Formula:	C17H24O
SMILES:	C=CC(O)C#CC#CCC=CCCCCCCC
Mol. weight [g/mol]:	244.37
CAS:	81203-57-8

Physical Properties

Property code	Value	Unit	Source
gf	526.66	kJ/mol	Joback Method
hf	235.53	kJ/mol	Joback Method
hfus	45.52	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	3.847		Crippen Method
mcvol	230.460	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1997.00		NIST Webbook
rinpol	1997.00		NIST Webbook
tb	698.94	K	Joback Method
tc	894.23	K	Joback Method
tf	532.53	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.46	J/mol×K	698.94	Joback Method
cpg	631.94	J/mol×K	731.49	Joback Method
cpg	646.65	J/mol×K	764.04	Joback Method

cpg	660.62	J/mol×K	796.58	Joback Method
cpg	673.91	J/mol×K	829.13	Joback Method
cpg	686.56	J/mol×K	861.68	Joback Method
cpg	698.61	J/mol×K	894.23	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C81203578&Units=SI

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
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