Falcarinol

Other names:	(Z)-(-)-1,9-Heptadecadiene-4,6-diyne-3-ol Falcarinol (Z)-(-)-1,9-heptadecadiene-4,6-diyne-3-ol (9Z)-1,9-Heptadecadiene-4,6-diyn-3-ol, (-)- cis-(-)-Heptadeca-1,9-dien-4,6-diyn-3-ol (-)-Falcarinol Panaxynol (Z)-Falcarinol
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-ZHACJKMWSA-N
Formula:	C17H24O
SMILES:	C=CC(O)C#CC#CCC=CCCCCCCC
Mol. weight [g/mol]:	244.37
CAS:	21852-80-2

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	2042.00		NIST Webbook
rinpol	2038.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	2038.00		NIST Webbook
ripol	3086.00		NIST Webbook
ripol	3086.00		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: 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=C21852802&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume