Falcarindiol

Inchi: InChI=1S/C17H24O2/c1-3-5-6-7-8-9-10-14-17(19)15-12-11-13-16(18)4-2/h4,10,14,16-19
InchiKey: QWCNQXNAFCBLLV-OQDIJTRPSA-N
Formula: C17H24O2
SMILES: C=CC(O)C#CC#CC(O)C=CCCCCCCC
Mol. weight [g/mol]: 260.37
CAS: 55297-87-5

Physical Properties

Property code	Value	Unit	Source
gf	387.40	kJ/mol	Joback Method
hf	78.02	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	89.61	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	2.818		Crippen Method
mcvol	236.330	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
tb	790.68	K	Joback Method
tc	984.23	K	Joback Method
tf	578.35	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.89	J/mol×K	790.68	Joback Method
cpg	690.30	J/mol×K	822.94	Joback Method
cpg	703.06	J/mol×K	855.20	Joback Method
cpg	715.21	J/mol×K	887.45	Joback Method
cpg	726.79	J/mol×K	919.71	Joback Method
cpg	737.85	J/mol×K	951.97	Joback Method
cpg	748.44	J/mol×K	984.23	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=C55297875&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume