Fokienol

Other names: Fokienol [(E,E)-Farnesa-1,6,9,11-tetraen-3-ol]
Inchi: InChI=1S/C17H28O/c1-6-17(5,18)14-10-13-16(4)12-9-7-8-11-15(2)3/h6,8,11,13,18H,1-2,
InchiKey: XCTSDLUOCRRDLZ-YZLWMTBJSA-N
Formula: C17H28O
SMILES: C=CC(C)(O)CCC=C(C)CCCC=CC(=C)C
Mol. weight [g/mol]: 248.40

Physical Properties

Property code	Value	Unit	Source
gf	277.30	kJ/mol	Joback Method
hf	-89.47	kJ/mol	Joback Method
hfus	31.68	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.952		Crippen Method
mcvol	239.060	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	1577.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1583.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2187.00		NIST Webbook
ripol	2174.00		NIST Webbook
ripol	2172.00		NIST Webbook
ripol	2177.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2174.00		NIST Webbook
tb	678.75	K	Joback Method
tc	860.47	K	Joback Method
tf	302.99	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.93	J/mol×K	678.75	Joback Method
cpg	676.03	J/mol×K	709.04	Joback Method
cpg	691.28	J/mol×K	739.32	Joback Method
cpg	705.77	J/mol×K	769.61	Joback Method
cpg	719.55	J/mol×K	799.89	Joback Method
cpg	732.69	J/mol×K	830.18	Joback Method
cpg	745.27	J/mol×K	860.47	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=R193801&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

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