

Homosalate

Other names:	Benzoic acid, 2-hydroxy-, 3,3,5-trimethylcyclohexyl ester Salicylic acid, 3,3,5-trimethylcyclohexyl ester Heliopan Heliophan Homomenthyl salicylate 3,3,5-Trimethylcyclohexyl salicylate m-Homomenthyl salicylate Coppertone Filtersol "A" Homosalat 2-Hydroxybenzoic acid 3,3,5-trimethylcyclohexyl ester Filtrosol A Kemester HMS NSC 164918
Inchi:	InChI=1S/C16H22O3/c1-11-8-12(10-16(2,3)9-11)19-15(18)13-6-4-5-7-14(13)17/h4-7,11-
InchiKey:	WSSJONWNBBTCMG-UHFFFAOYSA-N
Formula:	C16H22O3
SMILES:	CC1CC(OC(=O)c2ccccc2O)CC(C)(C)C1
Mol. weight [g/mol]:	262.34
CAS:	118-56-9

Physical Properties

Property code	Value	Unit	Source
gf	-188.75	kJ/mol	Joback Method
hf	-530.27	kJ/mol	Joback Method
hfus	27.49	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.764		Crippen Method
mcvol	214.990	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpola	1903.80		NIST Webbook
tb	759.52	K	Joback Method
tc	1001.30	K	Joback Method
tf	503.18	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.08	J/mol×K	759.52	Joback Method
cpg	674.30	J/mol×K	799.82	Joback Method
cpg	692.72	J/mol×K	840.11	Joback Method
cpg	710.54	J/mol×K	880.41	Joback Method
cpg	727.97	J/mol×K	920.71	Joback Method
cpg	745.21	J/mol×K	961.01	Joback Method
cpg	762.48	J/mol×K	1001.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C118569&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

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