

3-Flavene

Inchi:	InChI=1S/C15H12O/c1-2-6-12(7-3-1)15-11-10-13-8-4-5-9-14(13)16-15/h1-11,15H
InchiKey:	TXZZTLRVXGOMAB-UHFFFAOYSA-N
Formula:	C15H12O
SMILES:	C1=CC(c2ccccc2)Oc2ccccc21
Mol. weight [g/mol]:	208.26

Physical Properties

Property code	Value	Unit	Source
gf	283.10	kJ/mol	Joback Method
hf	101.08	kJ/mol	Joback Method
hfus	27.54	kJ/mol	Joback Method
hvap	59.09	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.833		Crippen Method
mcvol	165.400	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinqol	1780.00		NIST Webbook
tb	638.06	K	Joback Method
tc	899.16	K	Joback Method
tf	365.92	K	Joback Method
vc	0.616	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.55	J/molxK	638.06	Joback Method
cpg	489.97	J/molxK	855.65	Joback Method
cpg	478.06	J/molxK	812.13	Joback Method
cpg	464.98	J/molxK	768.61	Joback Method
cpg	450.63	J/molxK	725.09	Joback Method
cpg	434.86	J/molxK	681.58	Joback Method
cpg	500.86	J/molxK	899.16	Joback Method
dvisc	0.0003050	Paxs	638.06	Joback Method
dvisc	0.0003680	Paxs	592.70	Joback Method

dvisc	0.0004582	Paxs	547.35	Joback Method
dvisc	0.0005935	Paxs	501.99	Joback Method
dvisc	0.0008092	Paxs	456.63	Joback Method
dvisc	0.0011815	Paxs	411.28	Joback Method
dvisc	0.0018947	Paxs	365.92	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=R525352&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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