

Daucalene

Inchi:	InChI=1S/C15H18/c1-10(2)13-8-6-12(4)15-9-11(3)5-7-14(13)15/h5-10H,1-4H3
InchiKey:	OQDGHUJJXGDBDZ-UHFFFAOYSA-N
Formula:	C15H18
SMILES:	<chem>Cc1ccc2c(C(C)C)ccc(C)c2c1</chem>
Mol. weight [g/mol]:	198.30

Physical Properties

Property code	Value	Unit	Source
gf	263.15	kJ/mol	Joback Method
hf	34.98	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.580		Crippen Method
mcvol	178.990	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinsol	1672.00		NIST Webbook
tb	602.76	K	Joback Method
tc	827.42	K	Joback Method
tf	340.49	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.16	J/molxK	602.76	Joback Method
cpg	514.60	J/molxK	789.98	Joback Method
cpg	501.39	J/molxK	752.54	Joback Method
cpg	487.31	J/molxK	715.09	Joback Method
cpg	472.29	J/molxK	677.65	Joback Method
cpg	456.26	J/molxK	640.20	Joback Method
cpg	526.98	J/molxK	827.42	Joback Method
dvisc	0.0002427	Paxs	602.76	Joback Method
dvisc	0.0002889	Paxs	559.05	Joback Method

dvisc	0.0003542	Paxs	515.34	Joback Method
dvisc	0.0004510	Paxs	471.62	Joback Method
dvisc	0.0006032	Paxs	427.91	Joback Method
dvisc	0.0008620	Paxs	384.20	Joback Method
dvisc	0.0013500	Paxs	340.49	Joback Method

Sources

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=R428187&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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