

Tetrahydroaidzein (cis or trans isomer), TMS

Inchi:	InChI=1S/C15H14O4/c16-10-3-1-9(2-4-10)13-8-19-14-7-11(17)5-6-12(14)15(13)18/h1-7,
InchiKey:	YOSDNAMJVOLJKI-UHFFFAOYSA-N
Formula:	C15H14O4
SMILES:	Oc1ccc(C2COc3cc(O)ccc3C2O)cc1
Mol. weight [g/mol]:	258.27

Physical Properties

Property code	Value	Unit	Source
gf	-200.63	kJ/mol	Joback Method
hf	-483.89	kJ/mol	Joback Method
hfus	43.04	kJ/mol	Joback Method
hvap	101.19	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.307		Crippen Method
mvol	187.310	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
rinpol	2605.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	887.65	K	Joback Method
tc	1135.50	K	Joback Method
tf	645.18	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.58	J/molxK	887.65	Joback Method
cpg	653.79	J/molxK	1094.19	Joback Method
cpg	640.54	J/molxK	1052.88	Joback Method
cpg	627.81	J/molxK	1011.58	Joback Method
cpg	615.38	J/molxK	970.27	Joback Method
cpg	603.04	J/molxK	928.96	Joback Method
cpg	667.75	J/molxK	1135.50	Joback Method
dvisc	0.0000001	Paxs	887.65	Joback Method

dvisc	0.0000002	Paxs	847.24	Joback Method
dvisc	0.0000004	Paxs	806.83	Joback Method
dvisc	0.0000006	Paxs	766.42	Joback Method
dvisc	0.0000011	Paxs	726.00	Joback Method
dvisc	0.0000022	Paxs	685.59	Joback Method
dvisc	0.0000046	Paxs	645.18	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=R261419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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