

# cis-Diallate

<b>Inchi:</b>	InChI=1S/C10H17Cl2NOS/c1-7(2)13(8(3)4)10(14)15-6-9(12)5-11/h5,7-8H,6H2,1-4H3/b9
<b>InchiKey:</b>	SPANOECCGNXGNR-WEVVVXLNSA-N
<b>Formula:</b>	C10H17Cl2NOS
<b>SMILES:</b>	CC(C)N(C(=O)SCC(Cl)=CCl)C(C)C
<b>Mol. weight [g/mol]:</b>	270.22
<b>CAS:</b>	17708-57-5

## Physical Properties

Property code	Value	Unit	Source
gf	91.23	kJ/mol	Joback Method
hf	-187.52	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	61.49	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.277		Crippen Method
mvol	199.840	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
ripol	2322.00		NIST Webbook
ripol	2322.00		NIST Webbook
tb	641.31	K	Joback Method
tc	857.18	K	Joback Method
tf	330.06	K	Joback Method
vc	0.741	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.54	J/mol×K	641.31	Joback Method
cpg	486.39	J/mol×K	677.29	Joback Method
cpg	499.32	J/mol×K	713.27	Joback Method
cpg	511.40	J/mol×K	749.25	Joback Method
cpg	522.66	J/mol×K	785.22	Joback Method
cpg	533.15	J/mol×K	821.20	Joback Method
cpg	542.93	J/mol×K	857.18	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17708575&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17708575&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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