

Diallyl pentasulfide

Inchi:	InChI=1S/C6H10S5/c1-3-5-7-9-11-10-8-6-4-2/h3-4H,1-2,5-6H2
InchiKey:	CPDTWYIIHJBBCB-UHFFFAOYSA-N
Formula:	C6H10S5
SMILES:	C=CCSSSSSCC=C
Mol. weight [g/mol]:	242.47

Physical Properties

Property code	Value	Unit	Source
gf	340.92	kJ/mol	Joback Method
hf	293.04	kJ/mol	Joback Method
hfus	29.39	kJ/mol	Joback Method
hvap	61.70	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.684		Crippen Method
mcvol	168.550	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
rinqol	1690.00		NIST Webbook
tb	673.94	K	Joback Method
tc	958.16	K	Joback Method
tf	325.86	K	Joback Method
vc	0.604	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.19	J/mol×K	673.94	Joback Method
cpg	361.43	J/mol×K	721.31	Joback Method
cpg	371.59	J/mol×K	768.68	Joback Method
cpg	380.64	J/mol×K	816.05	Joback Method
cpg	388.56	J/mol×K	863.42	Joback Method
cpg	395.32	J/mol×K	910.79	Joback Method
cpg	400.89	J/mol×K	958.16	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=R311801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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