

DIALLYL TETRASULPHIDE

Other names:	Diallyl tetrasulphide Diallyl tetrasulfide
Inchi:	InChI=1S/C6H10S4/c1-3-5-7-9-10-8-6-4-2/h3-4H,1-2,5-6H2
InchiKey:	RMKCQUWJDRTEHE-UHFFFAOYSA-N
Formula:	C6H10S4
SMILES:	C=CCSSSSCC=C
Mol. weight [g/mol]:	210.41

Physical Properties

Property code	Value	Unit	Source
hf	146.00	kJ/mol	Cheméo Relay (1.0)
hfus	25.26	kJ/mol	Joback Method
hvap	70.28	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
logp	4.036		Crippen Method
mcvol	152.200	ml/mol	McGowan Method
rinpol	1538.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1502.00		NIST Webbook
tb	552.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	307.19	J/mol×K	605.16	Joback Method
cpg	318.59	J/mol×K	649.38	Joback Method
cpg	329.14	J/mol×K	693.60	Joback Method
cpg	338.83	J/mol×K	737.81	Joback Method
cpg	347.65	J/mol×K	782.03	Joback Method
cpg	355.60	J/mol×K	826.25	Joback Method
cpg	362.67	J/mol×K	870.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2444497&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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