

Methylvinylxyethyl sulfide

Inchi:	InChI=1S/C5H10OS/c1-3-6-4-5-7-2/h3H,1,4-5H2,2H3
InchiKey:	AAOKKJCPGNXYLC-UHFFFAOYSA-N
Formula:	C5H10OS
SMILES:	C=COCCSC
Mol. weight [g/mol]:	118.20
CAS:	6607-53-0

Physical Properties

Property code	Value	Unit	Source
af	0.3661		Cheméo Relay (1.0)
hf	-129.86	kJ/mol	Cheméo Relay (1.0)
hfus	12.74	kJ/mol	Joback Method
hvap	41.67	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-0.70		Cheméo Relay (1.0)
logp	1.510		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	420.79	K	Cheméo Relay (1.0)
tc	598.15	K	Cheméo Relay (1.0)
tf	205.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.68	J/mol×K	401.68	Joback Method
cpg	185.78	J/mol×K	434.04	Joback Method
cpg	194.58	J/mol×K	466.40	Joback Method
cpg	203.07	J/mol×K	498.76	Joback Method
cpg	211.27	J/mol×K	531.12	Joback Method
cpg	219.16	J/mol×K	563.47	Joback Method
cpg	226.73	J/mol×K	595.83	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44276e+01
Coeff. B	-4.55083e+03
Temperature range (K), min.	316.00
Temperature range (K), max.	499.21

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
Joback Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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