

Methyl propyl pentasulfide

Other names:	propyl methyl pentasulfide
Inchi:	InChI=1S/C4H10S5/c1-3-4-6-8-9-7-5-2/h3-4H2,1-2H3
InchiKey:	RFDQTEOGCIIPEK-UHFFFAOYSA-N
Formula:	C4H10S5
SMILES:	CCCCSSSSC
Mol. weight [g/mol]:	218.45

Physical Properties

Property code	Value	Unit	Source
gf	148.40	kJ/mol	Joback Method
hf	83.46	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	58.58	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.352		Crippen Method
mcvol	148.970	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1588.00		NIST Webbook
tb	634.82	K	Joback Method
tc	920.89	K	Joback Method
tf	306.84	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.02	J/molxK	634.82	Joback Method
cpg	311.13	J/molxK	682.50	Joback Method
cpg	321.33	J/molxK	730.18	Joback Method
cpg	330.54	J/molxK	777.85	Joback Method
cpg	338.71	J/molxK	825.53	Joback Method
cpg	345.77	J/molxK	873.21	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=R53454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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