n-Propyl n-hexyl disulfide

Other names: Propyl hexyl disulfide
Inchi: InChI=1S/C9H20S2/c1-3-5-6-7-9-11-10-8-4-2/h3-9H2,1-2H3
InchiKey: CKMPJNIZKDJPKH-UHFFFAOYSA-N
Formula: C9H20S2
SMILES: CCCCCCSSCCC
Mol. weight [g/mol]: 192.38
CAS: 64580-54-7

Physical Properties

Property code	Value	Unit	Source
gf	91.14	kJ/mol	Joback Method
hf	-145.35	kJ/mol	Joback Method
hfus	27.33	kJ/mol	Joback Method
hvap	49.26	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.358		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
ripol	1666.00		NIST Webbook
ripol	1666.00		NIST Webbook
tb	542.88	K	Joback Method
tc	745.83	K	Joback Method
tf	259.99	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.99	J/mol×K	542.88	Joback Method
cpg	402.36	J/mol×K	576.71	Joback Method
cpg	417.01	J/mol×K	610.53	Joback Method
cpg	430.95	J/mol×K	644.36	Joback Method
cpg	444.19	J/mol×K	678.18	Joback Method
cpg	456.73	J/mol×K	712.01	Joback Method

cpg	468.59	J/mol×K	745.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64580547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume