

N-PENTYL N-HEXYL DISULPHIDE

Other names:	Pentyl hexyl disulfide
Inchi:	InChI=1S/C11H24S2/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-11H2,1-2H3
InchiKey:	BBRSAOQUYAEPBG-UHFFFAOYSA-N
Formula:	C11H24S2
SMILES:	CCCCCSCCCCC
Mol. weight [g/mol]:	220.45

Physical Properties

Property code	Value	Unit	Source
af	0.5619		Cheméo Relay (1.0)
gf	107.98	kJ/mol	Joback Method
hf	-222.30	kJ/mol	Cheméo Relay (1.0)
hfus	32.51	kJ/mol	Joback Method
hvap	75.71	kJ/mol	Cheméo Relay (1.0)
ie	8.28	eV	Cheméo Relay (1.0)
log10ws	-5.67		Cheméo Relay (1.0)
logp	5.138		Crippen Method
mcvol	198.550	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
ripol	1836.00		NIST Webbook
ripol	1836.00		NIST Webbook
tb	551.89	K	Cheméo Relay (1.0)
tc	735.00	K	Cheméo Relay (1.0)
tf	242.32	K	Cheméo Relay (1.0)
vc	0.752	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.79	J/mol×K	588.64	Joback Method
cpg	501.57	J/mol×K	621.52	Joback Method
cpg	517.54	J/mol×K	654.39	Joback Method
cpg	532.72	J/mol×K	687.27	Joback Method
cpg	547.12	J/mol×K	720.15	Joback Method

cpg	560.75	J/mol×K	753.03	Joback Method
cpg	573.63	J/mol×K	785.90	Joback Method

Sources

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.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93305738&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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