Disulfide, dipentyl

Other names:	6,7-Dithiadodecane
	Bis(1-pentyl) disulfide
	Diamyl disulfide
	Dipentyl disulfide
	Pentyl disulfide
	di-n-Amyl disulfide
	dipentyl disulphide
	n-Amyl disulfide
Inchi:	InChI=1S/C10H22S2/c1-3-5-7-9-11-12-10-8-6-4-2/h3-10H2,1-2H3
InchiKey:	YSQZSPCQDXHJDJ-UHFFFAOYSA-N
Formula:	C10H22S2
SMILES:	CCCCCSSCCCCC
Mol. weight [g/mol]:	206.41
CAS:	112-51-6

Physical Properties

Property code	Value	Unit	Source
gf	99.56	kJ/mol	Joback Method
hf	-165.99	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	71.10 ± 0.20	kJ/mol	NIST Webbook
log10ws	-4.77		Crippen Method
logp	4.748		Crippen Method
mcvol	184.460	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1480.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1492.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1746.00		NIST Webbook
tb	565.76	K	Joback Method
tc	765.78	K	Joback Method
tf	271.26	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.14	J/mol×K	732.45	Joback Method
cpg	435.05	J/mol×K	565.76	Joback Method
cpg	451.18	J/mol×K	599.10	Joback Method
cpg	466.54	J/mol×K	632.43	Joback Method
cpg	481.15	J/mol×K	665.77	Joback Method
cpg	495.01	J/mol×K	699.11	Joback Method
cpg	520.55	J/mol×K	765.78	Joback Method
hvapt	59.80	kJ/mol	490.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.20	K	0.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48424e+01
Coeff. B	-4.58034e+03
Coeff. C	-9.04530e+01
Temperature range (K), min.	405.15
Temperature range (K), max.	571.03

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=C112516&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume