Methyl n-hexyl disulfide

Other names: Hexyl methyl disulfide
Inchi: InChI=1S/C7H16S2/c1-3-4-5-6-7-9-8-2/h3-7H2,1-2H3
InchiKey: WZUAZKYWEVGSEC-UHFFFAOYSA-N
Formula: C7H16S2
SMILES: CCCCCCSSC
Mol. weight [g/mol]: 164.33
CAS: 64580-52-5

Physical Properties

Property code	Value	Unit	Source
gf	74.30	kJ/mol	Joback Method
hf	-104.07	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	44.81	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.578		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
ripol	1605.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1540.00		NIST Webbook
tb	497.12	K	Joback Method
tc	706.23	K	Joback Method
tf	237.45	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.36	J/mol×K	497.12	Joback Method
cpg	309.83	J/mol×K	531.97	Joback Method
cpg	322.69	J/mol×K	566.82	Joback Method
cpg	334.95	J/mol×K	601.67	Joback Method
cpg	346.61	J/mol×K	636.52	Joback Method

cpg	357.67	J/mol×K	671.38	Joback Method
cpg	368.15	J/mol×K	706.23	Joback Method

Sources

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=C64580525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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