Dicyclohexylsulphide

Other names:	Cyclohexane, 1,1'-thiobis-
	Dicyclohexyl sulfide
Inchi:	InChI=1S/C12H22S/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h11-12H,1-10H2
InchiKey:	FTAORUVBXKFVDA-UHFFFAOYSA-N
Formula:	C12H22S
SMILES:	C1CCC(SC2CCCCC2)CC1
Mol. weight [g/mol]:	198.37
CAS:	7133-46-2

Physical Properties

Property code	Value	Unit	Source
gf	132.18	kJ/mol	Joback Method
hf	-140.50	kJ/mol	Joback Method
hfus	0.00	kJ/mol	Possible precursors and products of deep hydrodesulfurization of gasoline and distillate fuels IV. Heat capacities, enthalpy increments, vapor pressures, and derived thermodynamic functions for dicyclohexylsulfide between the temperatures (5 and 520) K
hvap	69.00 ± 0.70	kJ/mol	NIST Webbook
log10ws	-4.74		Crippen Method
logp	4.385		Crippen Method
mcvol	174.570	ml/mol	McGowan Method
pc	2370.00 ± 200.00	kPa	NIST Webbook
rhoc	283.47 ± 7.93	kg/m3	NIST Webbook
tb	581.84	K	Joback Method
tc	770.00 ± 6.00	K	NIST Webbook
tf	274.16	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.85	J/mol×K	834.84	Joback Method
cpg	480.58	J/mol×K	624.01	Joback Method
cpg	504.51	J/mol×K	666.17	Joback Method
cpg	526.65	J/mol×K	708.34	Joback Method
cpg	547.05	J/mol×K	750.50	Joback Method
cpg	565.76	J/mol×K	792.67	Joback Method
cpg	454.79	J/mol×K	581.84	Joback Method
hfust	5.68	kJ/mol	284.20	NIST Webbook
hvapt	65.40 ± 0.20	kJ/mol	429.00	NIST Webbook
hvapt	62.50 ± 0.10	kJ/mol	429.00	NIST Webbook
hvapt	59.50 ± 0.10	kJ/mol	429.00	NIST Webbook
hvapt	56.60 ± 0.10	kJ/mol	429.00	NIST Webbook
hvapt	53.70 ± 0.10	kJ/mol	429.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7133462&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Possible precursors and products of deep hydrodesulfurization of gasoline and distillate fuels IV. Heat capacities, enthalpy increments, vapor pressures, and derived thermodynamic functions for dicyclohexylsulfide between the temperatures (5 and 520) K: https://www.doi.org/10.1016/j.jct.2003.11.012

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hfust: Enthalpy of fusion at a given temperature
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
rhoc: Critical density

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