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]: 198.38

Physical Properties

Property code	Value	Unit	Source
hf	-172.14	kJ/mol	Cheméo Relay (1.0)
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
ie	8.22	eV	Cheméo Relay (1.0)
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	559.54	K	Cheméo Relay (1.0)
tc	770.00 ± 6.00	K	NIST Webbook
tf	298.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.65	J/mol×K	708.34	Joback Method
cpg	454.79	J/mol×K	581.84	Joback Method

cpg	480.58	J/mol×K	624.01	Joback Method
cpg	504.51	J/mol×K	666.17	Joback Method
cpg	547.05	J/mol×K	750.50	Joback Method
cpg	565.76	J/mol×K	792.67	Joback Method
cpg	582.85	J/mol×K	834.84	Joback Method
hfust	5.68	kJ/mol	284.20	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
hvapt	65.40 ± 0.20	kJ/mol	429.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7133462&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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