MESO-3,4-DICYCLOHEXYL-2,5-DIMETHYLHEXAN

Other names: Cyclohexane, 1,1'-(1,2-diethyl-1,2-dimethyl-1,2-ethanediyl)bis-, (R*,S*)-
(2-Cyclohexyl-1-isopropyl-3-methylbutyl)cyclohexane, meso-
Meso-3,4-dicyclohexyl-2,5-dimethylhexan
Inchi: InChI=1S/C20H38/c1-15(2)19(17-11-7-5-8-12-17)20(16(3)4)18-13-9-6-10-14-18/h15-20H
InchiKey: FBRPCXVEEDWFMC-UHFFFAOYSA-N
Formula: C20H38
SMILES: CC(C)C(C1CCCCC1)C(C(C)C)C1CCCCC1
Mol. weight [g/mol]: 278.52

Physical Properties

Property code	Value	Unit	Source
af	0.4842		Cheméo Relay (1.0)
chs	-12887.20 ± 1.80	kJ/mol	NIST Webbook
hf	-300.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-412.70 ± 1.80	kJ/mol	NIST Webbook
hfus	17.13	kJ/mol	Joback Method
hsub	112.70	kJ/mol	NIST Webbook
hvap	79.05	kJ/mol	Cheméo Relay (1.0)
ie	9.16	eV	Cheméo Relay (1.0)
logp	6.691		Crippen Method
mcvol	270.940	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
tb	608.32	K	Cheméo Relay (1.0)
tc	814.20	K	Cheméo Relay (1.0)
tf	295.86	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.00	J/mol×K	694.34	Joback Method
cpg	867.26	J/mol×K	730.67	Joback Method
cpg	893.66	J/mol×K	767.00	Joback Method
cpg	918.27	J/mol×K	803.33	Joback Method
cpg	941.16	J/mol×K	839.67	Joback Method

cpg	962.40	J/mol×K	876.00	Joback Method
cpg	982.07	J/mol×K	912.33	Joback Method
dvisc	0.0281491	Pa×s	269.92	Joback Method
dvisc	0.0038281	Pa×s	340.66	Joback Method
dvisc	0.0010339	Pa×s	411.39	Joback Method
dvisc	0.0004100	Pa×s	482.13	Joback Method
dvisc	0.0002060	Pa×s	552.87	Joback Method
dvisc	0.0001210	Pa×s	623.60	Joback Method
dvisc	0.0000792	Pa×s	694.34	Joback Method
hsubt	113.00 ± 2.10	kJ/mol	343.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62678528&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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hsub: Enthalpy of sublimation at standard conditions

hsubt: Enthalpy of sublimation at a given temperature

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point