1,1,3-Tricyclohexylpropane

Other names: Cyclohexane, 1,1',1''-(1-propanyl-2-ylidene)tris-
Propane, 1,1,3-tricyclohexyl-
Inchi: InChI=1S/C21H38/c1-4-10-18(11-5-1)16-17-21(19-12-6-2-7-13-19)20-14-8-3-9-15-20/h18
InchiKey: VIDXNEQHNUTDHC-UHFFFAOYSA-N
Formula: C21H38
SMILES: C1CCC(CCC(C2CCCCC2)C2CCCCC2)CC1
Mol. weight [g/mol]: 290.53
CAS: 55682-89-8

Physical Properties

Property code	Value	Unit	Source
gf	196.85	kJ/mol	Joback Method
hf	-319.09	kJ/mol	Joback Method
hfus	22.13	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	7.124		Crippen Method
mcvol	274.170	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
tb	738.09	K	Joback Method
tc	973.24	K	Joback Method
tf	333.57	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1046.25	J/mol×K	973.24	Joback Method
cpg	1026.79	J/mol×K	934.05	Joback Method
cpg	1005.44	J/mol×K	894.85	Joback Method
cpg	982.10	J/mol×K	855.66	Joback Method
cpg	956.67	J/mol×K	816.47	Joback Method
cpg	929.05	J/mol×K	777.28	Joback Method
cpg	899.16	J/mol×K	738.09	Joback Method

cpl	638.10	J/mol×K	373.00	NIST Webbook
dvisc	0.0001317	Pa×s	670.67	Joback Method
dvisc	0.0002065	Pa×s	603.25	Joback Method
dvisc	0.0003626	Pa×s	535.83	Joback Method
dvisc	0.0007485	Pa×s	468.41	Joback Method
dvisc	0.0019717	Pa×s	400.99	Joback Method
dvisc	0.0076831	Pa×s	333.57	Joback Method
dvisc	0.0000912	Pa×s	738.09	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55682898&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.