Cyclododecene

Other names: Cyclododecene,c&t
Cyclododecene (c,t)
Inchi: InChI=1S/C12H22/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-2H,3-12H2
InchiKey: HYPABJGVBDSCIT-UHFFFAOYSA-N
Formula: C12H22
SMILES: C1=CCCCCCCCCCC1
Mol. weight [g/mol]: 166.30
CAS: 1501-82-2

Physical Properties

Property code	Value	Unit	Source
gf	39.68	kJ/mol	Joback Method
hf	-195.53	kJ/mol	Joback Method
hfus	6.22	kJ/mol	Joback Method
hvap	44.37	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.457		Crippen Method
mcvol	164.780	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1291.00		NIST Webbook
rinpol	1315.00		NIST Webbook
tb	511.70	K	NIST Webbook
tb	511.50 ± 6.50	K	NIST Webbook
tc	765.93	K	Joback Method
tf	216.26	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.42	J/mol×K	522.96	Joback Method
cpg	410.08	J/mol×K	563.46	Joback Method
cpg	435.15	J/mol×K	603.95	Joback Method
cpg	458.64	J/mol×K	644.45	Joback Method

cpg	480.53	J/mol×K	684.94	Joback Method
cpg	500.83	J/mol×K	725.44	Joback Method
cpg	519.53	J/mol×K	765.93	Joback Method
dvisc	0.1989191	Pa×s	216.26	Joback Method
dvisc	0.0140649	Pa×s	267.38	Joback Method
dvisc	0.0023276	Pa×s	318.49	Joback Method
dvisc	0.0006335	Pa×s	369.61	Joback Method
dvisc	0.0002366	Pa×s	420.73	Joback Method
dvisc	0.0001094	Pa×s	471.84	Joback Method
dvisc	0.0000588	Pa×s	522.96	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1501822&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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