n-Dodecylcyclopentane

Other names: DODECYLCYCLOPENTANE
Inchi: InChI=1S/C17H34/c1-2-3-4-5-6-7-8-9-10-11-14-17-15-12-13-16-17/h17H,2-16H2,1H3
InchiKey: UFGYKQGTOYNLLD-UHFFFAOYSA-N
Formula: C17H34
SMILES: CCCCCCCCCCCCC1CCCC1
Mol. weight [g/mol]: 238.45
CAS: 5634-30-0

Physical Properties

Property code	Value	Unit	Source
af	0.6690		KDB
chl	-11215.80 ± 2.50	kJ/mol	NIST Webbook
gf	126.00	kJ/mol	KDB
hf	-336.10	kJ/mol	KDB
hf	-333.20 ± 2.70	kJ/mol	NIST Webbook
hfus	33.72	kJ/mol	Joback Method
hvap	85.50	kJ/mol	NIST Webbook
log10ws	-6.59		Crippen Method
logp	6.488		Crippen Method
mcvol	239.530	ml/mol	McGowan Method
pc	1400.00	kPa	KDB
tb	584.10	K	KDB
tc	755.20	K	KDB
tf	265.70 ± 1.00	K	NIST Webbook
tf	265.70 ± 0.50	K	NIST Webbook
tf	268.00	K	KDB
vc	0.928	m3/kmol	KDB
zc	0.2070200		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.30	J/mol×K	692.06	Joback Method
cpg	776.38	J/mol×K	780.48	Joback Method

cpg	759.25	J/mol×K	751.01	Joback Method
cpg	741.24	J/mol×K	721.54	Joback Method
cpg	659.63	J/mol×K	603.64	Joback Method
cpg	681.53	J/mol×K	633.11	Joback Method
cpg	702.41	J/mol×K	662.59	Joback Method
dvisc	0.0001919	Pa×s	603.64	Joback Method
dvisc	0.0005480	Pa×s	447.94	Joback Method
dvisc	0.0003592	Pa×s	499.84	Joback Method
dvisc	0.0002550	Pa×s	551.74	Joback Method
dvisc	0.0047853	Pa×s	292.25	Joback Method
dvisc	0.0018689	Pa×s	344.15	Joback Method
dvisc	0.0009339	Pa×s	396.05	Joback Method
hvapt	68.00	kJ/mol	534.50	NIST Webbook
hvapt	52.59	kJ/mol	584.10	KDB
rhol	816.00	kg/m3	293.00	KDB
srf	0.03	N/m	298.20	KDB

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5634300&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

KDB: https://www.cheric.org/files/research/kdb/mol/mol599.mol

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

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

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

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
rhol:	Liquid Density
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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