Cadinane

Inchi: InChI=1S/C15H28/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h10-15H,5-9H2,1-4H3/t1
InchiKey: FZZNNPQZDRVKLU-HGSUQPQSSA-N
Formula: C15H28
SMILES: CC1CCC2C(C)CCC(C(C)C)C2C1
Mol. weight [g/mol]: 208.38

Physical Properties

Property code	Value	Unit	Source
gf	122.95	kJ/mol	Joback Method
hf	-298.27	kJ/mol	Joback Method
hfus	22.17	kJ/mol	Joback Method
hvap	48.18	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.741		Crippen Method
mcvol	200.490	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1483.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1618.00		NIST Webbook
tb	558.71	K	Joback Method
tc	767.90	K	Joback Method
tf	252.89	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.96	J/mol×K	558.71	Joback Method
cpg	567.48	J/mol×K	593.57	Joback Method
cpg	592.55	J/mol×K	628.44	Joback Method

cpg	616.21	J/mol×K	663.30	Joback Method
cpg	638.49	J/mol×K	698.17	Joback Method
cpg	659.45	J/mol×K	733.03	Joback Method
cpg	679.13	J/mol×K	767.90	Joback Method
dvisc	0.0025609	Pa×s	252.89	Joback Method
dvisc	0.0014675	Pa×s	303.86	Joback Method
dvisc	0.0009869	Pa×s	354.83	Joback Method
dvisc	0.0007332	Pa×s	405.80	Joback Method
dvisc	0.0005821	Pa×s	456.77	Joback Method
dvisc	0.0004840	Pa×s	507.74	Joback Method
dvisc	0.0004163	Pa×s	558.71	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R134144&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume