Cadinane-b

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
InchiKey: FZZNNPQZDRVKLU-UHFFFAOYSA-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	1456.00		NIST Webbook
rinpol	1457.00		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	659.45	J/mol×K	733.03	Joback Method
cpg	638.49	J/mol×K	698.17	Joback Method
cpg	616.21	J/mol×K	663.30	Joback Method
cpg	592.55	J/mol×K	628.44	Joback Method
cpg	567.48	J/mol×K	593.57	Joback Method
cpg	679.13	J/mol×K	767.90	Joback Method
dvisc	0.0004163	Pa×s	558.71	Joback Method

dvisc	0.0004840	Pa×s	507.74	Joback Method
dvisc	0.0005821	Pa×s	456.77	Joback Method
dvisc	0.0007332	Pa×s	405.80	Joback Method
dvisc	0.0009869	Pa×s	354.83	Joback Method
dvisc	0.0014675	Pa×s	303.86	Joback Method
dvisc	0.0025609	Pa×s	252.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R306502&Units=SI

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