2-butylideneadamantane

Inchi: InChI=1S/C14H22/c1-2-3-4-14-12-6-10-5-11(8-12)9-13(14)7-10/h4,10-13H,2-3,5-9H2,1H
InchiKey: QYYRVPQXQWMSSI-CPSFFCFKSA-N
Formula: C14H22
SMILES: CCCC=C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	274.90	kJ/mol	Joback Method
hf	-64.36	kJ/mol	Joback Method
hfus	25.71	kJ/mol	Joback Method
hvap	47.15	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.169		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1454.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1648.00		NIST Webbook
tb	546.18	K	Joback Method
tc	754.37	K	Joback Method
tf	303.96	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.21	J/mol×K	546.18	Joback Method

cpg	473.88	J/mol×K	580.88	Joback Method
cpg	494.17	J/mol×K	615.58	Joback Method
cpg	513.17	J/mol×K	650.27	Joback Method
cpg	530.99	J/mol×K	684.97	Joback Method
cpg	547.72	J/mol×K	719.67	Joback Method
cpg	563.46	J/mol×K	754.37	Joback Method
dvisc	0.0013639	Pa×s	303.96	Joback Method
dvisc	0.0013981	Pa×s	344.33	Joback Method
dvisc	0.0014257	Pa×s	384.70	Joback Method
dvisc	0.0014485	Pa×s	425.07	Joback Method
dvisc	0.0014676	Pa×s	465.44	Joback Method
dvisc	0.0014838	Pa×s	505.81	Joback Method
dvisc	0.0014978	Pa×s	546.18	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R304531&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
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