2-n-butyladamantane

Other names: 2-Butyladamantane
Inchi: InChI=1S/C14H24/c1-2-3-4-14-12-6-10-5-11(8-12)9-13(14)7-10/h10-14H,2-9H2,1H3
InchiKey: ZOQLCQXGZZFWAF-UHFFFAOYSA-N
Formula: C14H24
SMILES: CCCCC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 192.34
CAS: 14449-43-5

Physical Properties

Property code	Value	Unit	Source
gf	221.73	kJ/mol	Joback Method
hf	-160.73	kJ/mol	Joback Method
hfus	26.46	kJ/mol	Joback Method
hvap	46.05	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.249		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1499.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1651.00		NIST Webbook
tb	534.87	K	Joback Method
tc	736.34	K	Joback Method

tf	289.36	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.33	J/mol×K	534.87	Joback Method
cpg	492.49	J/mol×K	568.45	Joback Method
cpg	514.26	J/mol×K	602.03	Joback Method
cpg	534.73	J/mol×K	635.61	Joback Method
cpg	553.97	J/mol×K	669.19	Joback Method
cpg	572.08	J/mol×K	702.77	Joback Method
cpg	589.13	J/mol×K	736.34	Joback Method
dvisc	0.0012460	Pa×s	289.36	Joback Method
dvisc	0.0013579	Pa×s	330.28	Joback Method
dvisc	0.0014520	Pa×s	371.20	Joback Method
dvisc	0.0015322	Pa×s	412.12	Joback Method
dvisc	0.0016011	Pa×s	453.03	Joback Method
dvisc	0.0016610	Pa×s	493.95	Joback Method
dvisc	0.0017135	Pa×s	534.87	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=C14449435&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume